Unscrambler X
Process Pulse

User Manual

Version 1.1

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1 Introduction

Unscrambler X Process Pulse was designed to be an easy to use and versatile software package for real time monitoring of processes utilizing a wide range of process analysis equipment. Combining the power of multivariate models with intuitive plot configurations and automatic alarm systems Unscrambler X Process Pulse is an invaluable tool for detecting and correcting deviations from target process conditions. Process monitoring is based on models for prediction or classification previously trained and validated using The Unscrambler® X multivariate analysis software. The state of a process or product quality attributes can be measured in real-time with equipment such as process spectrometers or other process analysis inputs.

Unscrambler X Process Pulse supports most of the common data formats, both vendor-specific and generic. It can be connected via OPC or through a Programmable Logic Controller (PLC) using communication protocols such as TCP/IP etc. A set of pre-specified diagnostic plots can be configured and displayed on a computer screen or other Human Machine Interface (HMI) and updated as new samples are being measured. These plots can be used by process operators or quality assurance to identify any anomalous or deviating samples, while interactive drill-down options enable detailed investigations of raw data. The prediction and classification results, as well as a list of any deviating samples, are written to output folders for subsequent investigation and analysis. A flow chart is provided in Figure 1 depicting a typical workflow.

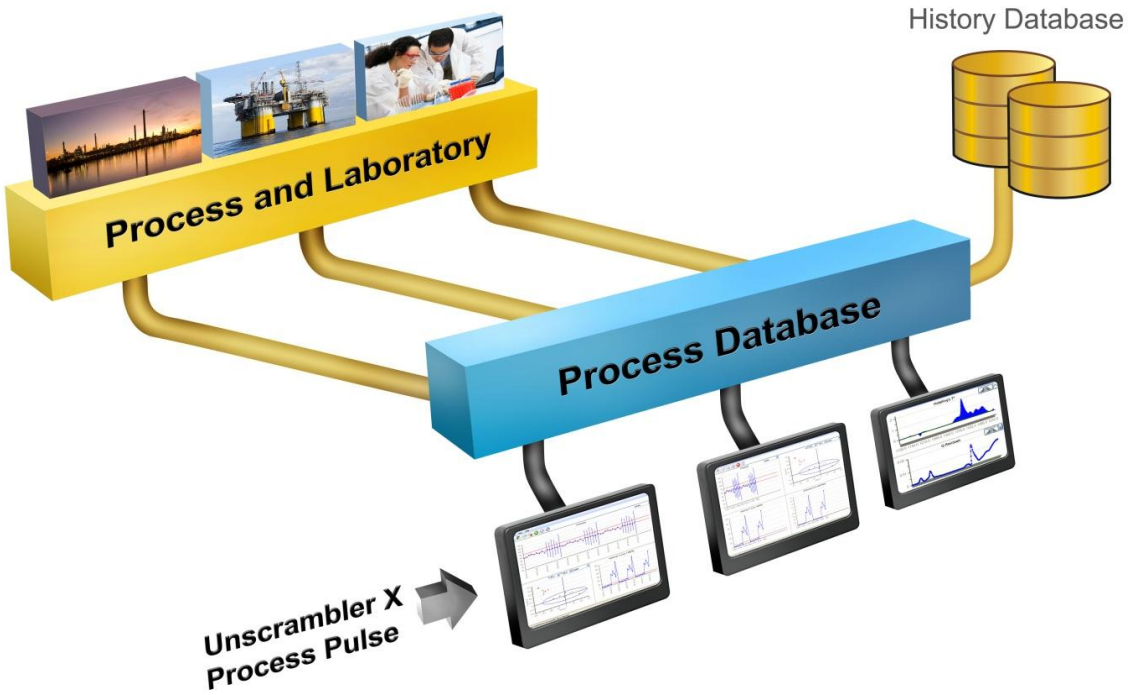

Figure 1 - Data Flow Chart

1.1 Assumptions and General Statements Regarding Unscrambler X Process Pulse

For the purposes of setting up configuration methods in Unscrambler X Process Pulse, the reader of this document should have a sound working knowledge of multivariate predictive and classification models used for real time analysis purposes and in particular, should have worked with The Unscrambler® X product.

Routine users of the program do not necessarily need a full working knowledge of multivariate modeling but should be familiar with the output and plot interpretation associated with each plot.

Unscrambler X Process Pulse is a simple *monitoring* tool for general process applications and in of itself is not a *control* system. However, it is customizable to specific user requirements and the outputs generated can be used by third party systems for control applications. Contact your local CAMO Software office for more details on customization of the package.

1.2 Typographic Conventions

Throughout this document, the following typographic conventions are followed.

- *A User* is defined as a person who uses the Unscrambler® X multivariate analysis software and/or Unscrambler X Process Pulse software.

- A *Configuration method* is a pre-defined list of instructions for performing a prediction, classification or projection routine. The configuration methods contain the multivariate models developed in The Unscrambler® for real time prediction and classification purposes.

- The *Configuration navigator* is a side pane in the main startup screen that contains the configuration methods available to a user for the application of real time prediction, classification and projection models to new data.

2 Getting Started

This section describes the general usage of Unscrambler X Process Pulse software package.

2.1 Package Contents

Unscrambler X Process Pulse installer comes with the file **UnscramblerXProcessPulseSetUp.msi**. This file is used for installing the program.

A step-by-step installation procedure is provided that guides a user through the setup and activation of the software.

Please Note: An installation and operational qualification document is available for the setup procedure. Please contact CAMO Software if you require this document.

3 Application Startup

After successful installation of the software, launch the application by double clicking on the application icon available on the desktop or by clicking on Unscrambler X Process Pulse 1.0 menu from programs list. An activation key will be requested when the application is launched for the first time.

3.1 Activation dialog

Upon launching the application for the first time, an activation dialog will appear (see Figure 2). Users with a working internet connection may use the **Obtain** button to request an activation key online. Make sure the fields **Machine ID**, **Name** and **Company** are correctly filled in. A user may also contact their local CAMO office directly to obtain the activation key.

Figure 2 - Activation Dialog

3.2 Login dialog

Once the software is activated, a login screen will be displayed upon startup (see Figure 3). The default and recommended option is to log on using windows authentication credentials. This will provide a traceable signature stamp in the audit trail contained within the software.

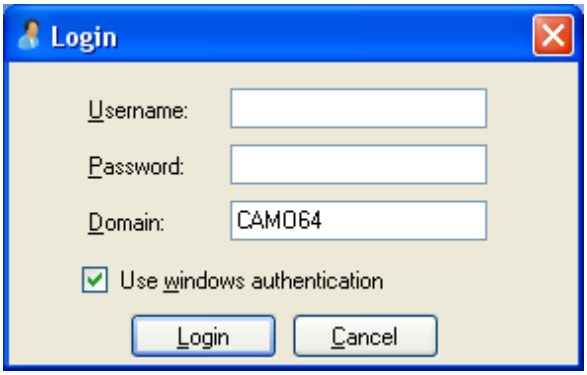

Figure 3 - Default Login Dialog

For testing purposes or other situations where traceability is not required, the *windows authentication* option may be de-selected and the user may log on as Guest. A warning will be displayed as shown in Figure 4 stating the data will be collected in non-compliance mode.

Figure 4 - Guest Login Dialog

A splash screen with the program branding and version details will appear for approximately 3 seconds when the **Login** button is selected. After this, the user will be taken to the *Startup Screen*.

3.3 Startup Screen

The startup screen is shown in Figure 5. In addition to the main work space, a list of configurations is displayed on the left side pane (if any have been previously configured) called the *configuration navigator*. A pane for *configuration info* is displayed at the bottom of the screen, and a set of menu items and tools are provided at the top of the screen. If the program has been installed for the first time, no *configuration methods* will be displayed in the *configuration navigator*.

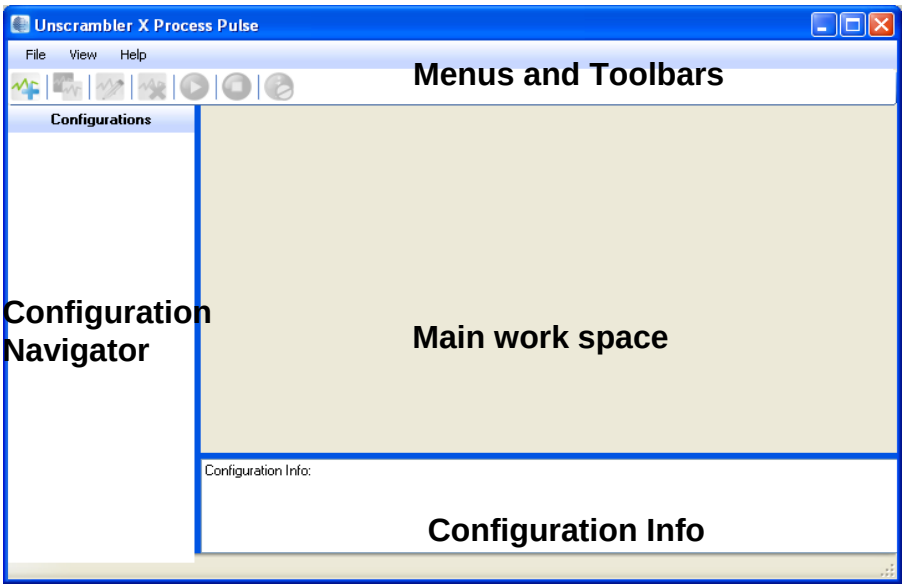

Figure 5 - Startup Screen

3.4 Configuration Method Setup

In order to use Unscrambler X Process Pulse application for prediction and/or classification and/or projection purposes, the following are essential:

- The Unscrambler® X model(s)
- File path location for storing the samples from a data source (spectrometer or other)
- File path location for storing the results of prediction or classification or projection routines.

A file that stores these parameters is referred to as a *configuration method*.

Unscrambler X Process Pulse facilitates *creation* of new configuration methods, along with the abilities to *modify*, *duplicate* and *delete* existing configuration methods. Section 3.4.1 describes how to set up configuration methods for predictive models and section 3.4.2 describes the corresponding procedure for classification models.

3.4.1 Creating a Configuration Method for Prediction

To create a new configuration method, click on the **New** button ( ) in the toolbar or select the menu **File -> Configuration-> New** to start the setup wizard. The options for creating a new configuration method are shown in Figure 6.

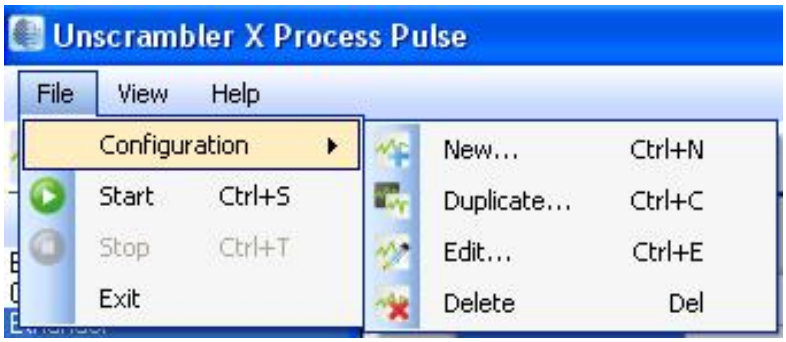

Figure 6 - New Configuration Menu option

The *Create Configuration* dialog screen, as shown in Figure 7, will appear. Select *Prediction* by clicking in the radio button at the top of the dialog. Enter a *Configuration Name*. Configuration method names can be any alphanumeric text (including some special characters like underscore '_', hyphen '-'and opening and closing brackets '('and ')'), but not a space character. This will also be the name given to the *Output* folder where results will be stored.

Follow through the tabs and provide the required input information for a particular configuration method. This is described in more details in the following sections.

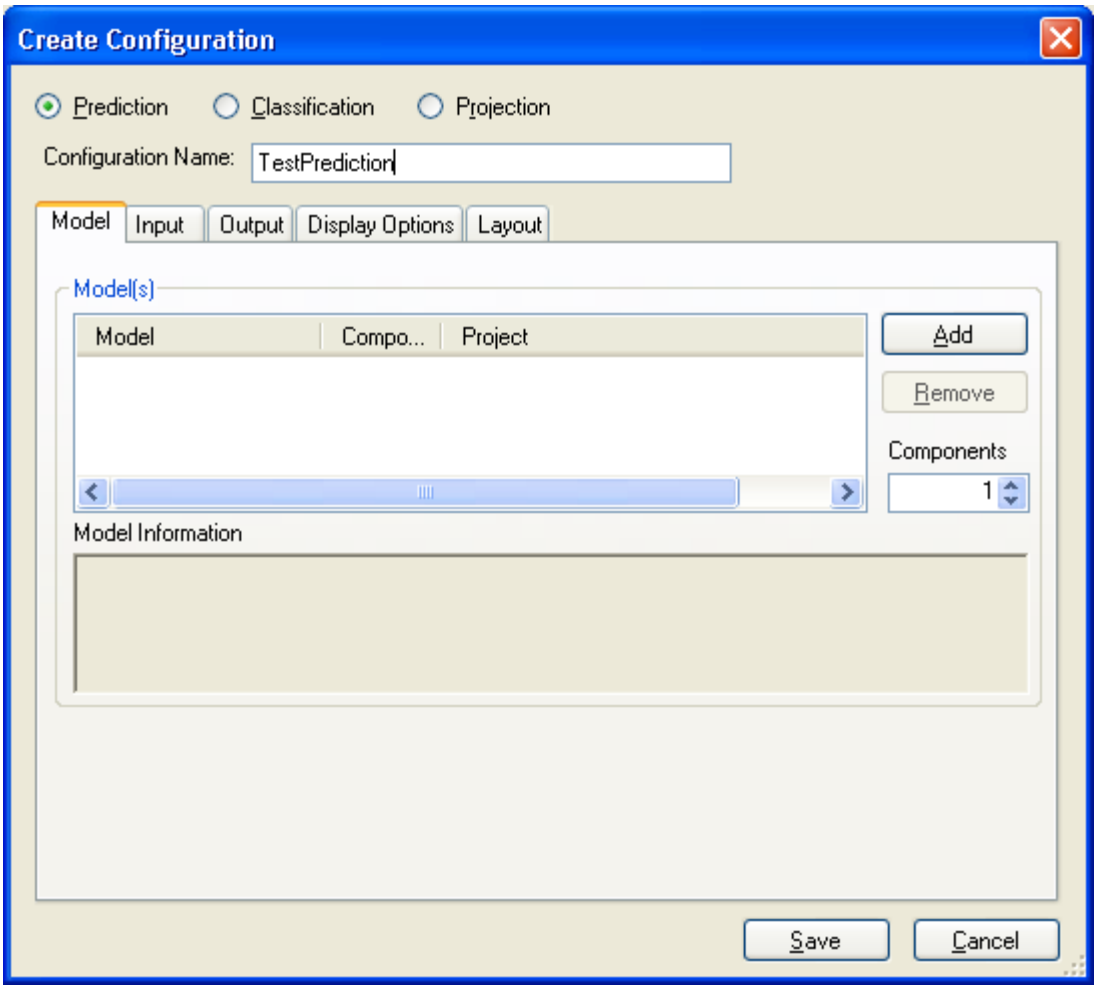

Figure 7 - Configuration Dialog

The Model Tab

The Unscrambler® X model files that are to be used for prediction are specified in the *Model* tab (See Figure 7). Only one model can be loaded and used for prediction per configuration method (*however, if a PLS model with multiple constituents can be used*). Each sample that is read in during the prediction process is predicted using the model that is selected in the configuration method. New input data should have the same number of variables as that used to develop the original calibration model and read in using the same order as specified in the model. For this reason, models developed for instrumental data should have all the variables, and use the *Keep outs* option in The Unscrambler® X range definition dialog to exclude columns from the analysis rather than deleting columns from the input data when the model is developed.

The Add Button

To enter an Unscrambler® X model, click on the **Add** button. The *Select Model* dialog (as shown in Figure 8) will appear where an Unscrambler® X project or model file can be entered, or use the **Browse** button to find a project/file in a specific directory (a standard Windows file selection dialog appears that can be browsed to the directory containing the project or model files). An example of this dialog is shown in Figure 9.

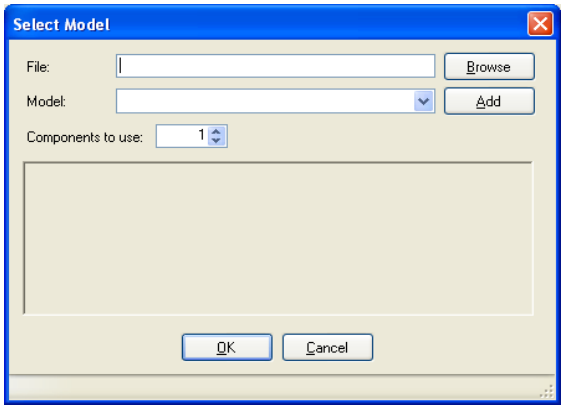

Figure 8 - Select Model Dialog

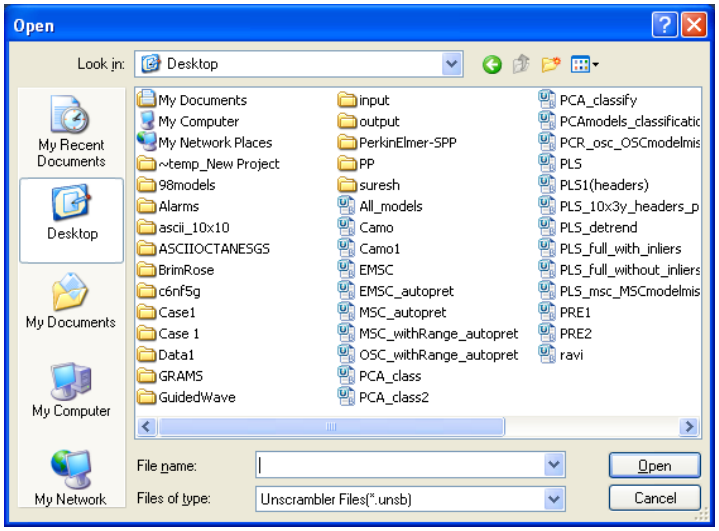

Figure 9 - Open Dialog for selecting Models

If the Unscrambler® X project file is password protected an *Enter Password* dialog (shown in Figure 10) will appear. On entering the correct password, a user can see the list of models in the selected project file (see Figure 11).

Figure 10 - Password dialog

All models in a project will be accessible from the *Model* drop-down box. Select the appropriate model from the list and view the model information displayed for the selected model (see Figure 11). Click on the **Add** button to configure the Prediction method.

Note*:* Only valid models (full PLS, PCR or MLR models) can be added here.

Upto three models can be loaded for prediction purposes. Please contact your local CAMO Software office if a greater number of models is required for a particular application.

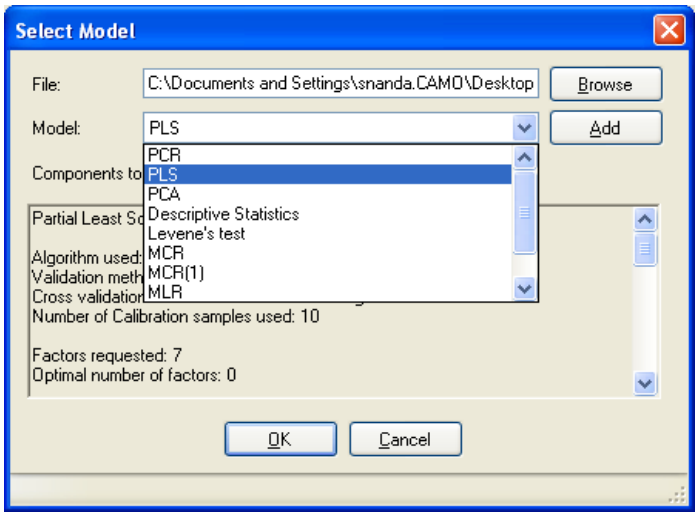

Figure 11 - Select Model

The Remove button

Models can be removed from the list by selecting the model from the *Model(s)* list, and clicking the **Remove** button. The selected model is removed from the list.

Components

The number of components to be used for prediction is shown in the *Components* numeric spin box. The optimum number of components for a model is suggested based on information in the Unscrambler® X model file, however this may be modified by the user (provided the components were not previously saved to a model in The Unscrambler® X)

Model Information

Information about the currently highlighted model is displayed in the *Model Information* section.

The Input tab

Directory

The sample files generated during the process (i.e. from the process equipment, spectrometer etc.) are to be saved into a directory specified here. When the configuration method and process are started, input sample files are read from this folder and used for prediction purposes. A **Browse** button can be used to specify the input directory. An example is provided in Figure 12.

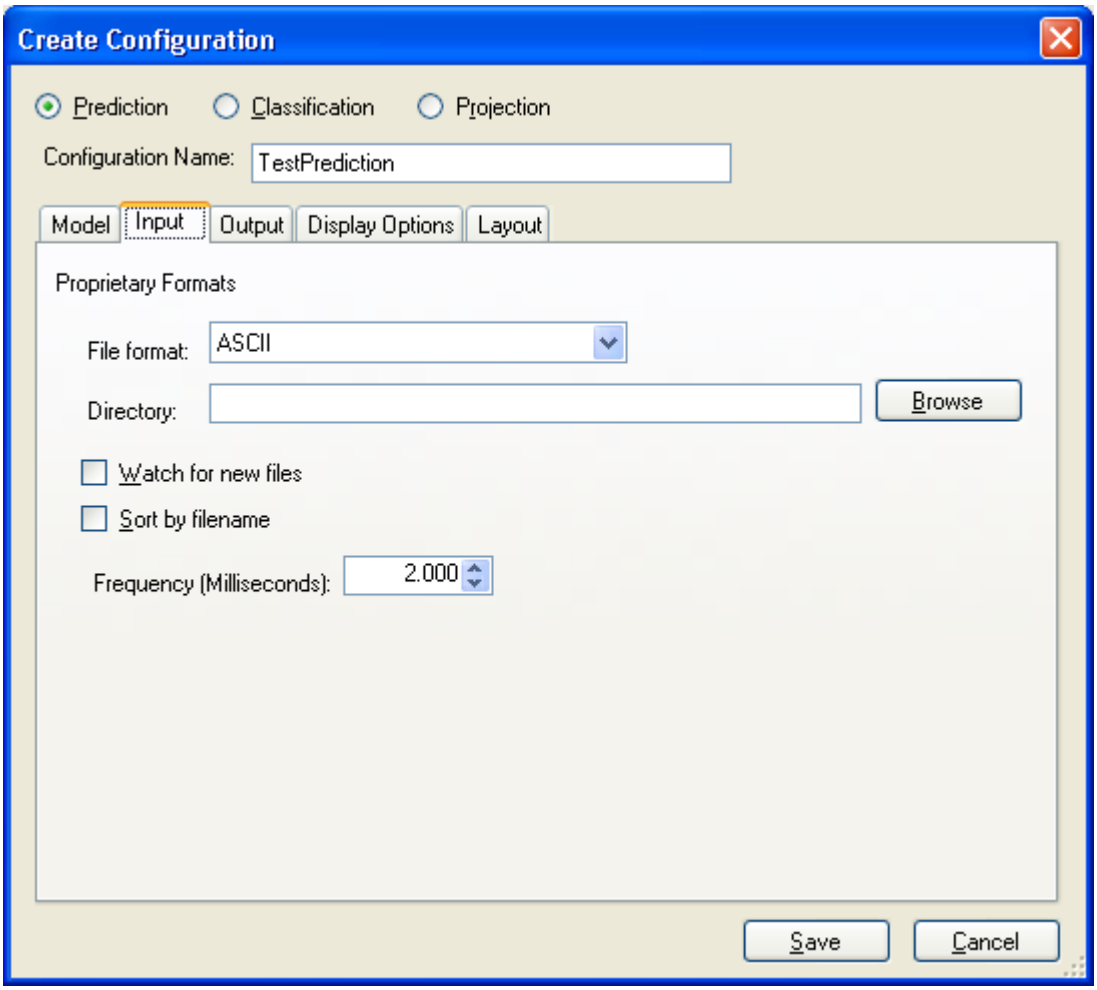

Figure 12 - Input tab

File Format

The file format of the input files is specified in the *File format* drop-down box. The file formats supported in Unscrambler X Process Pulse are provided in Table 1.

Table 1 - File Formats supported

OEM Name	Format	Supported File Extensions
Most of the instrument vendors	JCAMPDX	*.jdx,*.dx,*.jcm,*.jx,*.jxs
THERMO	GRAMS	*.spc,*.cfl
BRIMROSE	BFF3, BFF4	*.dat
ASD Inc	INDICO	*.asd,*.asf,*.001
VARIAN	Cary UV-Vis	*.BSW
Bruker	OPUS	*.0x, *.01
Thermo	OMNIC	*.spa,*.spg
Guided Wave	SpectrOn , ClassPA	*.asc, *.scn, *.data, *.gva, *.updated, etc
Foss	NSAS	*.da,*.DA
Perkin Elmer	Spectrum 6, Spectrum 10	*.sp,*.spp
	ASCII	*.txt,*.csv
	Excel	*.xls,*.xlsx

Watch for New Files

If this option is set the prediction process is notified whenever a new file is added to the *Input* directory. The new file is loaded and processed once any previous predictions have been completed.

This option is for the so called *asynchronous mode* of operation. When this mode is set the other two options, *Sort by file name* and *Frequency* cannot be set and become inactive.

Sort by File Name

If this option is set, all files located in the *Input* directory are sorted and loaded sequentially in alphabetical order. Application of the prediction method is done on this sorted order.

Frequency

The numeric *Frequency* box can be used to provide the frequency (in milliseconds) at which the application should poll the *Input* directory for new and existing input data.

The Output tab

The location of predicted results produced after the application of a configuration method to new or existing data is defined in the *Output* tab. This tab also allows the pre-configuration of graphical outputs to be displayed for a configuration method. *Output* tab is shown in Figure 13.

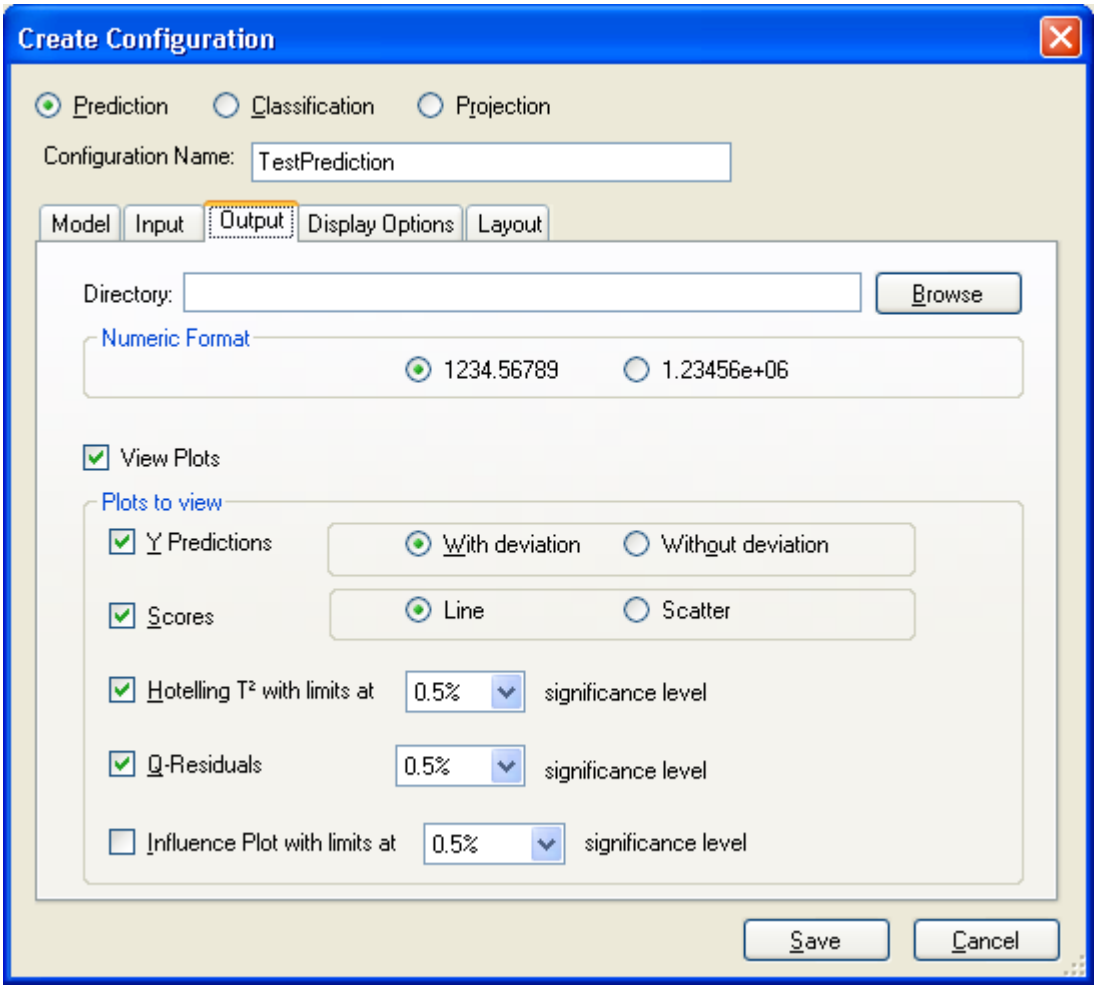

Figure 13 - Output Tab

Output directory

The *Output* directory provides the path for the output files. This includes three files in csv format for prediction: configuration summary, results, and alarms (in a subfolder).

Numeric Format

The *Numeric Format* box provides the option to print the numeric results in floating point format (12345.6789111) or exponential format (1.234568e+06). The selection defines how the results are written to the *Output* file.

Plots to view (Prediction Configuration Methods Only)

A user can select which diagnostic plot(s) to display during process monitoring. One or more of the following plots may be displayed

- Y-Predictions (with or without deviations)
- Scores (line or 2D-scatter plot)
- Hotelling's T^2-statistics with limits at a specified significance level

- Q-Residuals at a specified significance level
- Influence plot with limits at a specified significance level

Note: If the view plots option is selected, the plots are displayed during process monitoring, the outputs of projections are written directly in the output directory.

The Display Options tab

This tab is available for prediction configuration methods only. An example is provided in Figure 14.

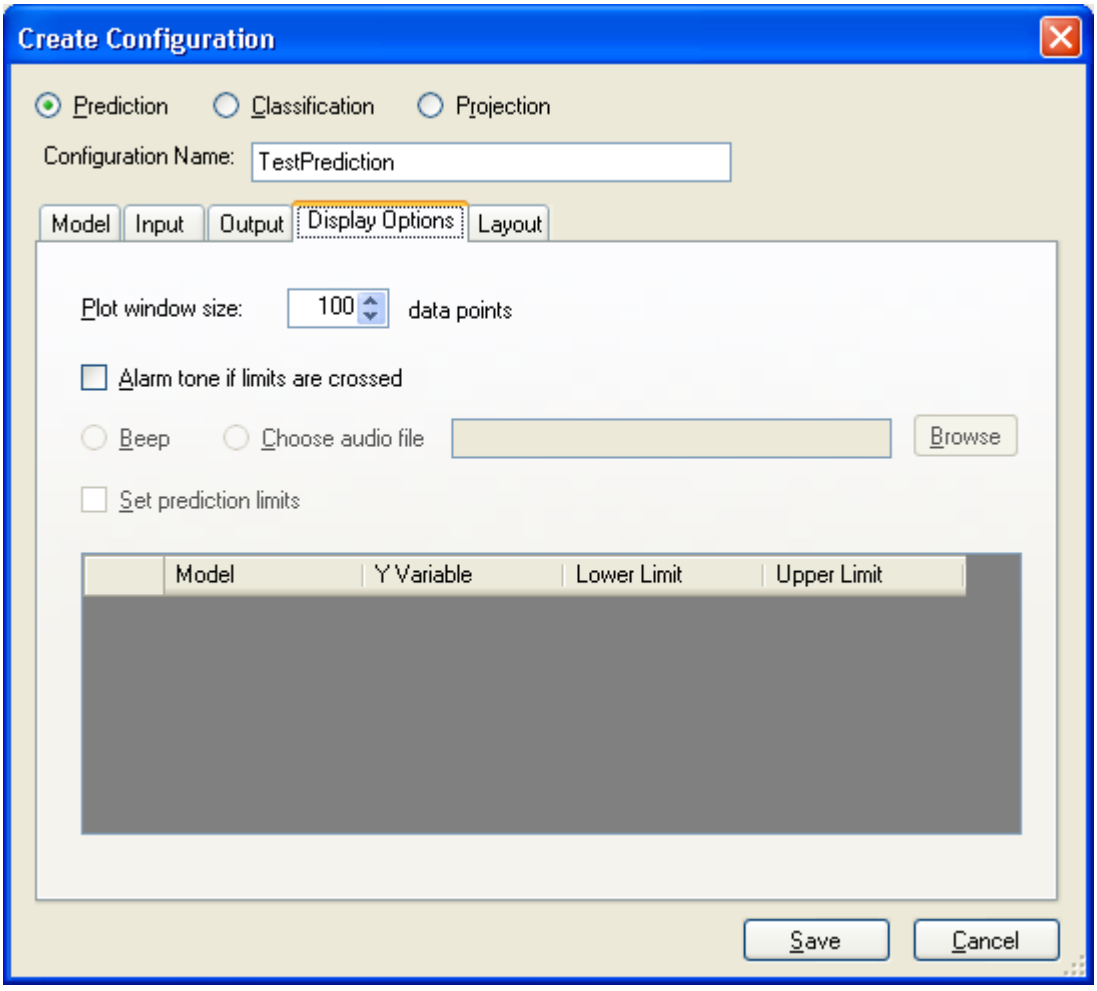

Figure 14 - Display options tab

Plot Window Size

The maximum number of data points to be displayed in the plots is defined here.

Alarm tone if Limits Are Crossed

An audible alarm is sounded whenever the process deviates from target conditions if this option is selected. The alarm can be used from the Operating System beep sound or an audio file can be specified for alarm.

Set Prediction Limits

Control limits as defined by the user are entered in these fields, one for the lower control limit and one for the upper control limit. These limits are displayed in red in the Y-Predicted plots. If a predicted value falls outside of these limits an entry of the alert is written to the *Alarms file*.

The Layout tab

For configuration methods using prediction models, a user can select any layout from the list of nine shown in Figure 15. The layout should have the same number of panes as there are plots selected in the *Output* tab.

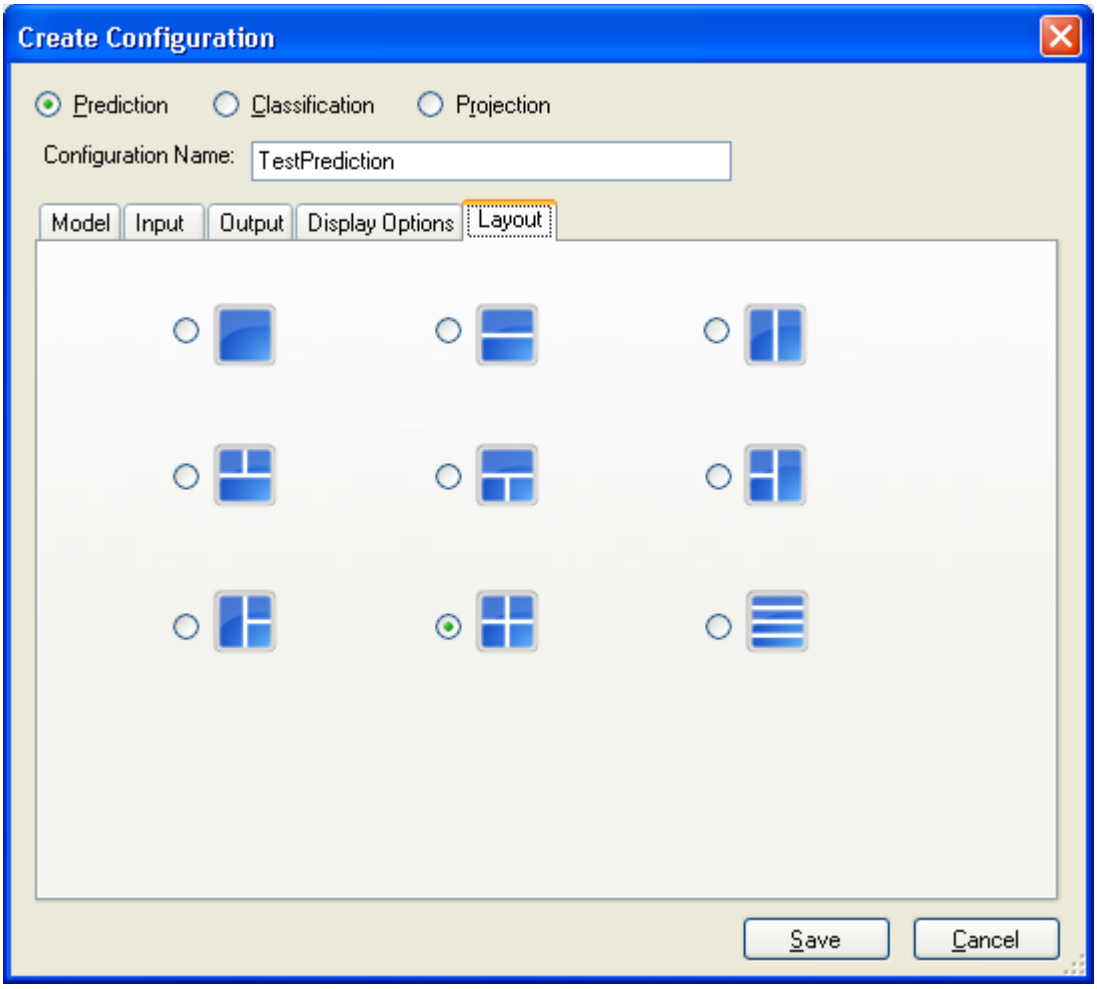

Figure 15 - Layout tab

Save Configuration Method

All of the settings (options) chosen by the user are saved as a *Configuration method*.

Configuration method names can be any alphanumeric text (including some special characters like underscore '_', hyphen '-'and opening and closing brackets '('and ')') but not a space character.

Click the **Save** button to save the configuration method into the *Configuration Navigator*. The configuration method appears in the configuration navigator with the name it was saved as.

3.4.2 Configuration Dialog for Classification Configuration Methods

The Model Tab

The Unscrambler® X model files that are to be used for classification are specified in the *Model* tab. Up to five models can be used for classification purposes. Each sample that is read into the *Input* directory during the process is classified using the specified model(s). See Figure 16 for an example.

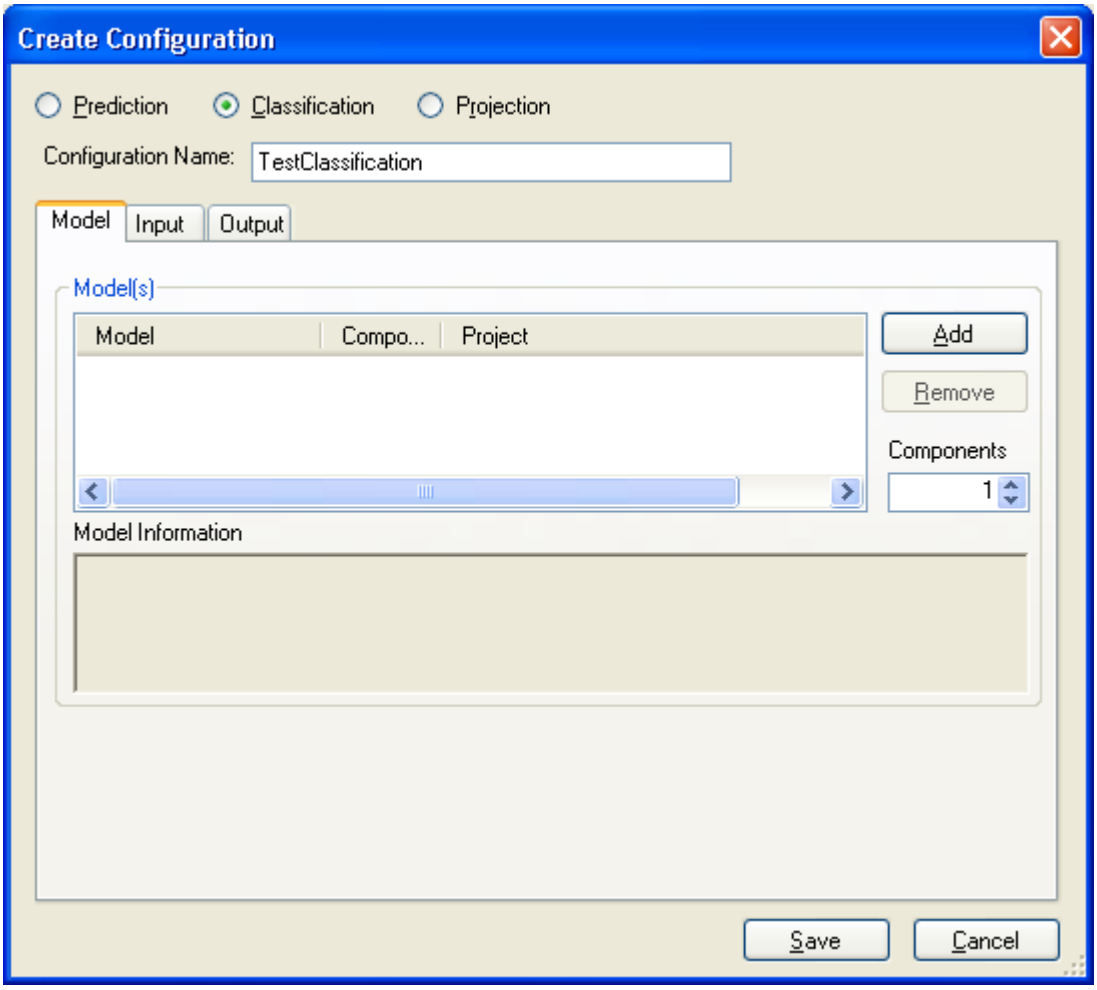

Figure 16 - Model tab for Classification

The Add Button

Click on the **Add** button. The *Select Model* dialog (as shown in Figure 17) will appear where a user can browse for Unscrambler® X project or model files (as shown in Figure 18). A standard windows file selection appears listing the files.

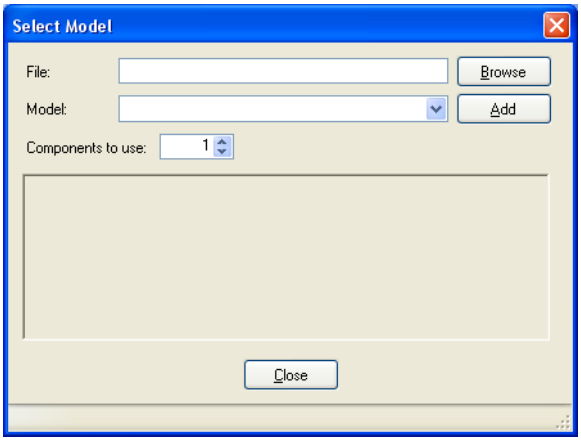

Figure 17 - Select Model Dialog

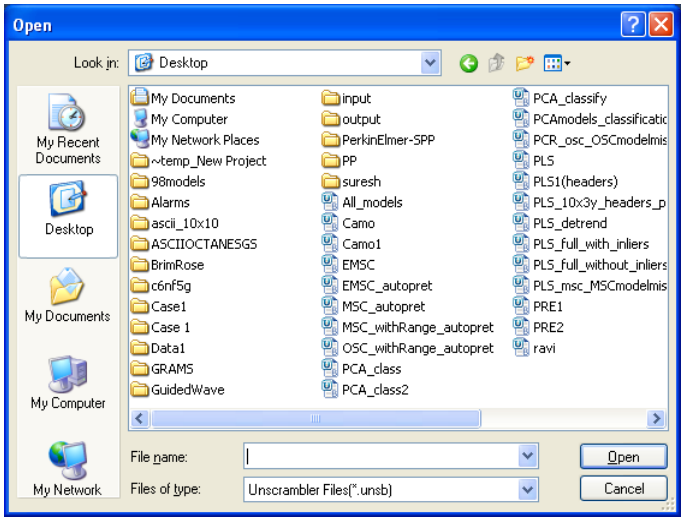

Figure 18 - Open Dialog for selecting Models

If The Unscrambler® X project file is password protected an *Enter Password* dialog box (shown in Figure 19) will appear. On entering the correct password, a user can see the list of models in the selected project file (see Figure 20).

Figure 19 - Password dialog

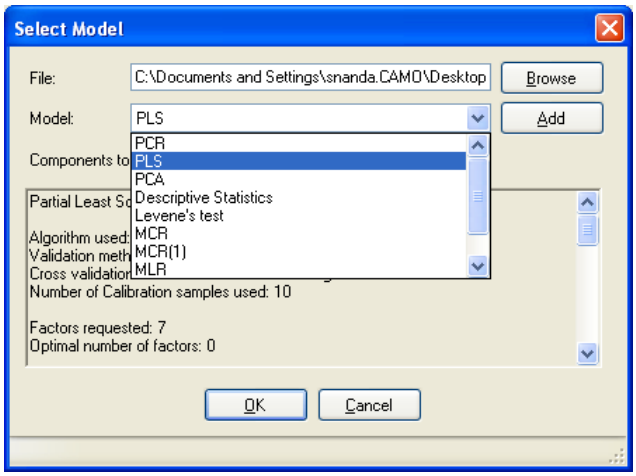

Figure 20 - Select Model

Select any model from the list and view the model information (see Figure 20). Click on the **Add** button to include the Classification model into the configuration method.

Note: Only valid models (Full PLS, PCR, PCA models) can be added here.

Up to five models can be loaded for classification purposes. Please contact your local CAMO Software office if a greater number of models are required for a particular application.

Remove button

Models can be removed from the list by selecting the model from the *Model(s)* list, and clicking the **Remove** button. The selected model is removed from the list.

Components

The number of components to be used for classification is shown in the *Components* numeric spin box. The optimum number of components for a model is suggested; however this may be modified by the user (provided the components were not previously saved to a model in The Unscrambler® X).

For classification configuration methods, the models must all have the same transformations and use the same number of variables.

Model Information

Information about the currently highlighted model is displayed in the *Model Information* section.

The Input tab

Directory

The sample files generated during a routine process analysis are found in a directory specified here. When the classification process starts, input sample files are read from this folder and used for classification. The *Input* tab is shown in Figure 21 for a classification configuration method. A **Browse** button can be used to specify the *Input* directory.

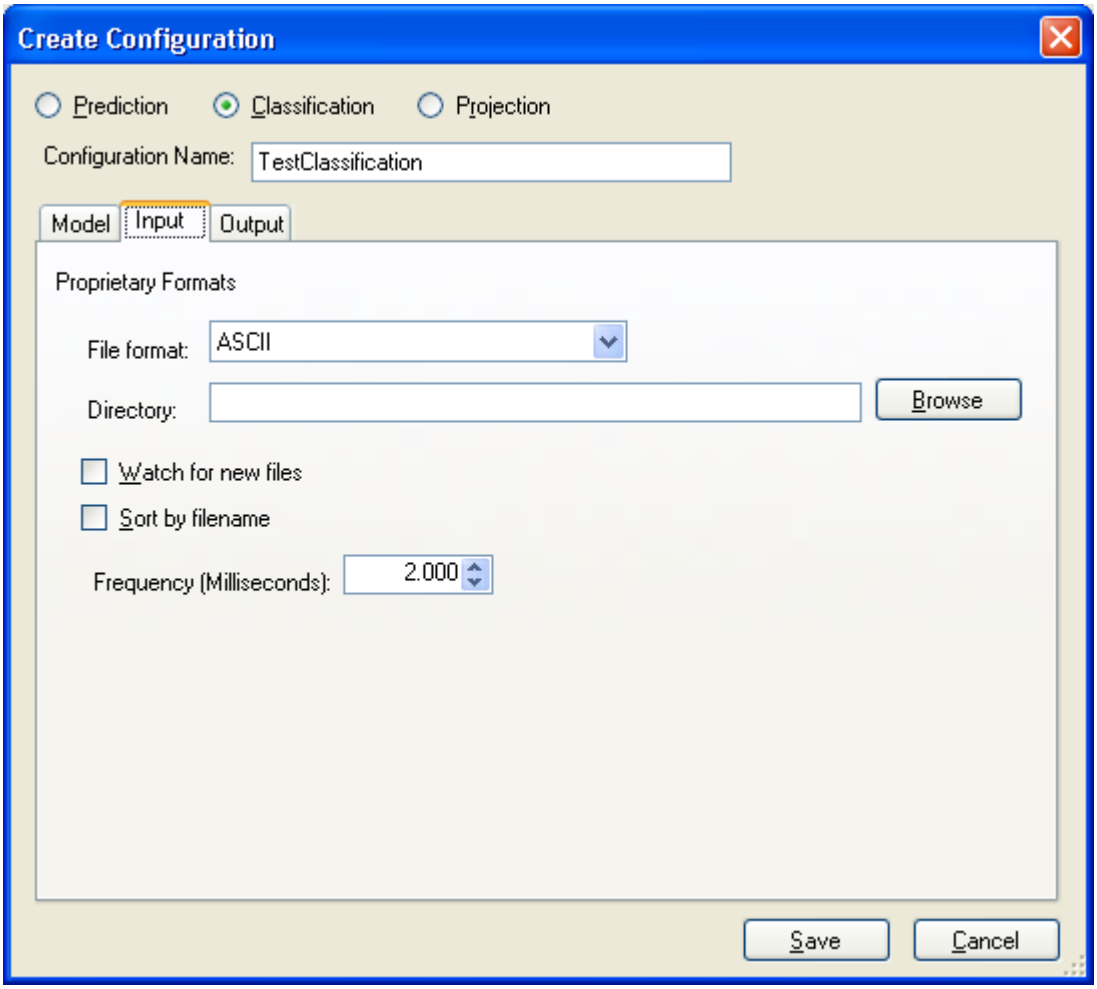

Figure 21 - Input tab for Classification

Watch for New Files

If this option is selected, the classification process is notified whenever a new file is added to the *Input* directory. The new file is loaded and processed once any previous classifications have been completed.

This option is for what is known as *asynchronous* mode of operation. When this mode is set the other two options, *Sort by file name* and *Frequency* cannot be set.

Sort by File Name

If this option is selected, all existing files in the *Input* directory are sorted and loaded sequentially in alphabetical order. Classification is performed on the samples in their sorted order.

Frequency

The numeric *Frequency* box can be used to provide the frequency (in milliseconds) at which the application should poll the *Input* directory for new data.

The Output tab

The information required for performing classification and storing the results are defined in the *Output* tab, (see Figure 22 for an example for a classification configuration method)

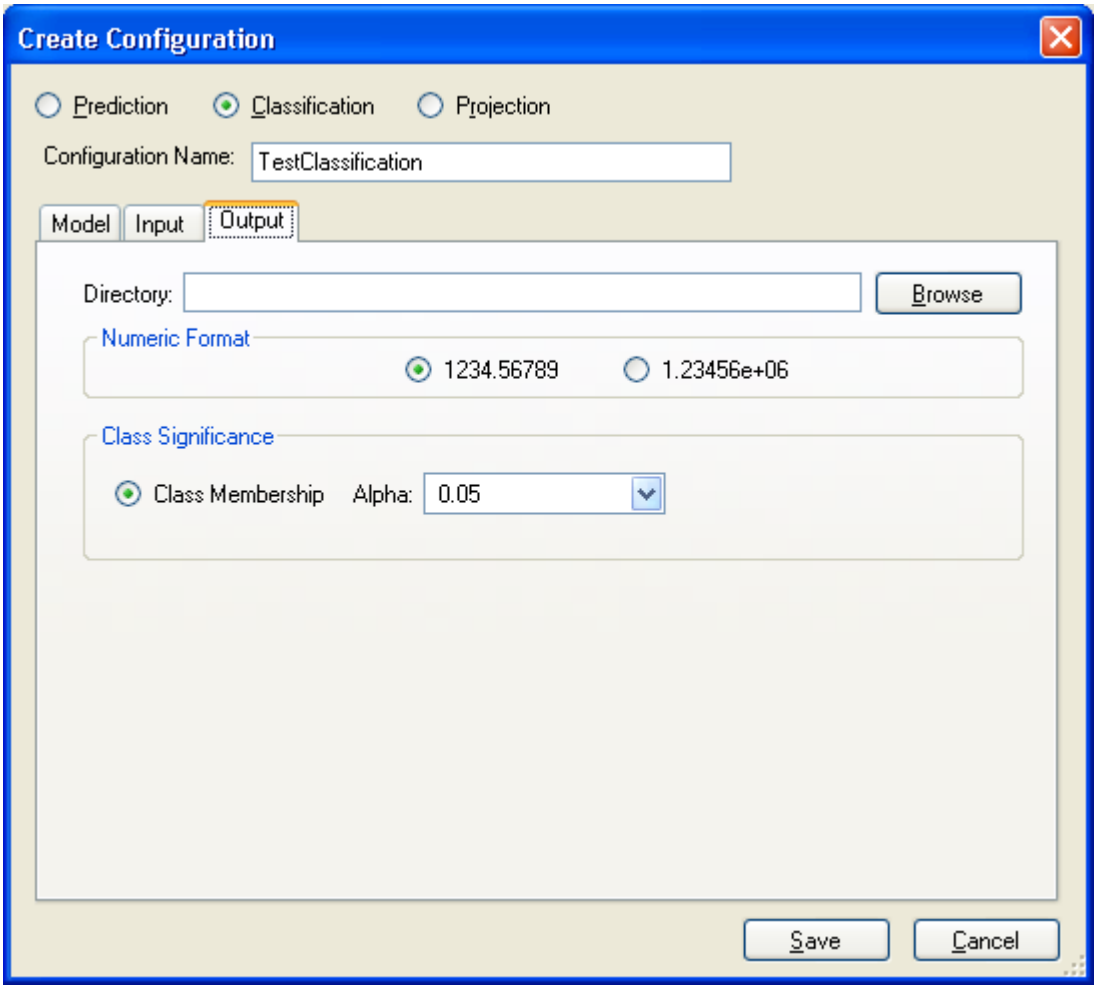

Figure 22 - Output Tab for Classification

Output directory

The *Output* directory defines the path for the output files which include the results file.

Numeric Format

The *Numeric Format* box provides the option to print the numeric results in floating point format (12345.6789111) or exponential format (1.234568e+06). Depending on the selection, the results are stored in floating point or scientific notation.

Class Significance

Here a user selects the significance level (alpha) for class membership from the drop-down menu. The default value is 0.05. See Figure 22.

3.4.3 Configuration Dialog for Projection Configuration Methods

The Model Tab

The Unscrambler® X model files that are to be used for projection are specified in the *Model* tab. Each sample that is read into the *Input* directory during the process is projected using the specified model. See Figure 23 for an example.

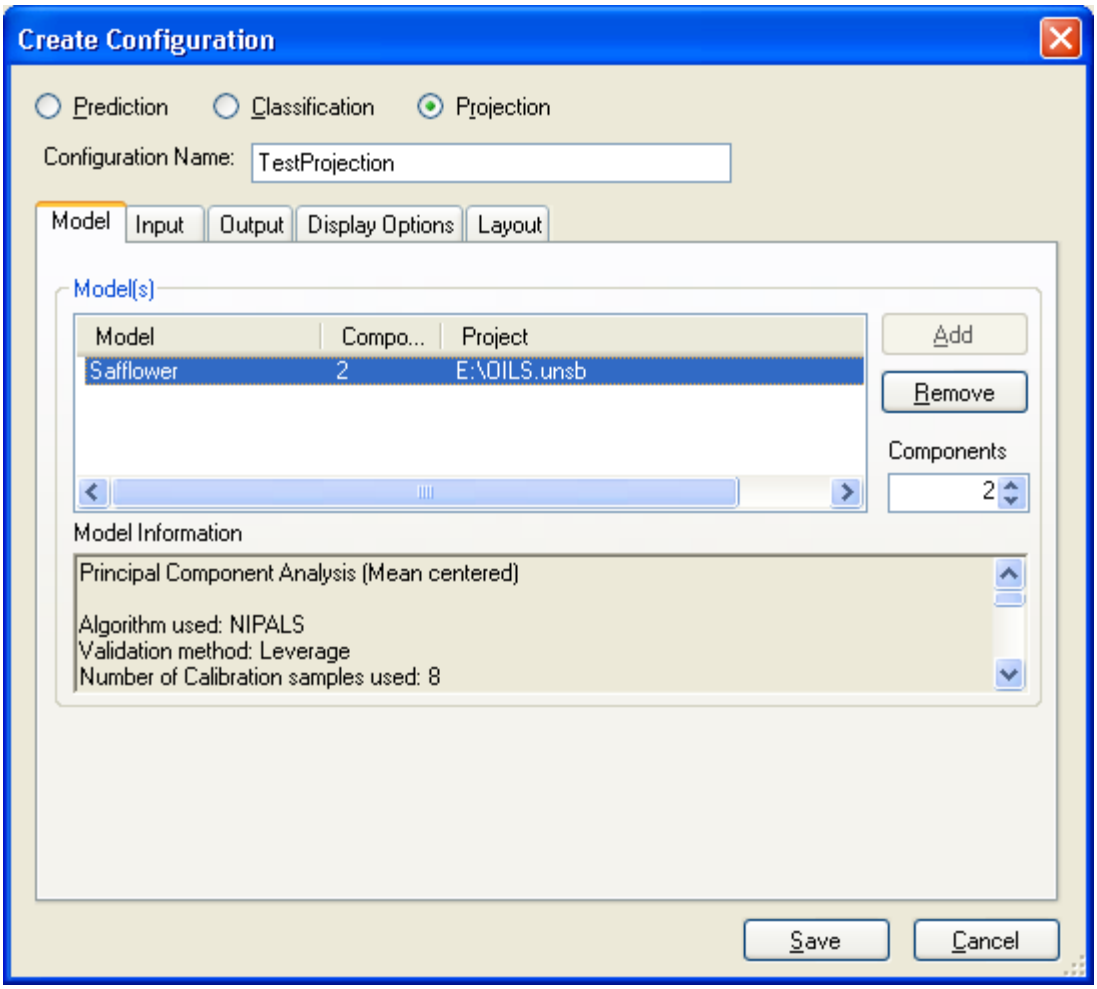

Figure 23 - Model tab for Projection

The Add Button

Click on the **Add** button. The *Select Model* dialog (as shown in Figure 17) will appear where a user can browse for Unscrambler® X project or model files (as shown in Figure 24). A standard windows file selection appears listing the files.

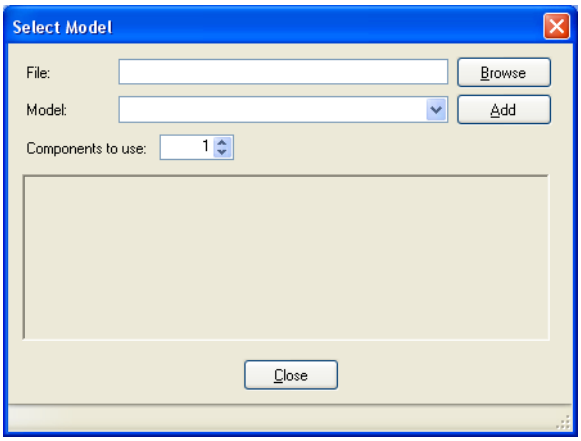

Figure 24 - Select Model Dialog

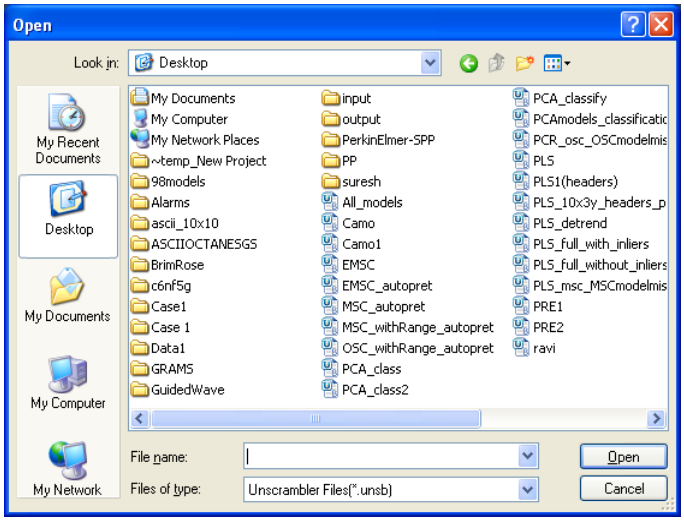

Figure 25 - Open Dialog for selecting Models

If The Unscrambler® X project file is password protected an *Enter Password* dialog box (shown in Figure 26) will appear. On entering the correct password, a user can see the list of models in the selected project file (see Figure 27).

Figure 26 - Password dialog

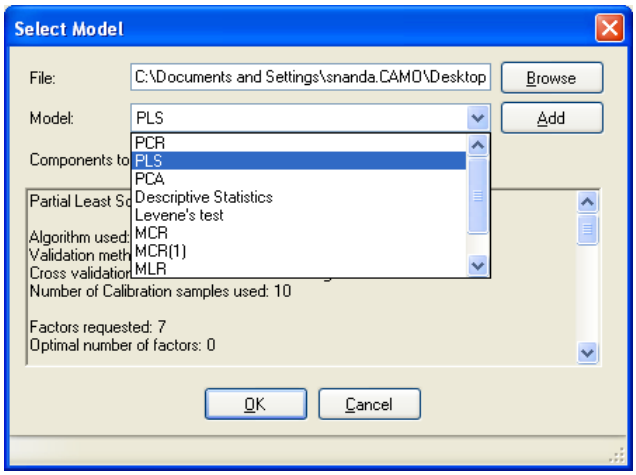

Figure 27 - Select Model

Select any model from the list and view the model information (see Figure 27). Click on the **Add** button to include the Projection model into the configuration method.

Note: Only valid models (Full PLS, PCR, PCA models) can be added here.

Remove button

Models can be removed from the list by selecting the model from the *Model(s)* list, and clicking the **Remove** button. The selected model is removed from the list.

Components

The number of components to be used for projection is shown in the *Components* numeric spin box. The optimum number of components for a model is suggested; however this may be modified by the user (provided the components were not previously saved to a model in The Unscrambler® X).

Model Information

Information about the currently highlighted model is displayed in the *Model Information* section.

The Input tab

Directory

The sample files generated during a routine process analysis are found in a directory specified here. When the projection process starts, input sample files are read from this folder and used for projection. The *Input* tab is shown in Figure 21 for a projection method. A **Browse** button can be used to specify the *Input* directory.

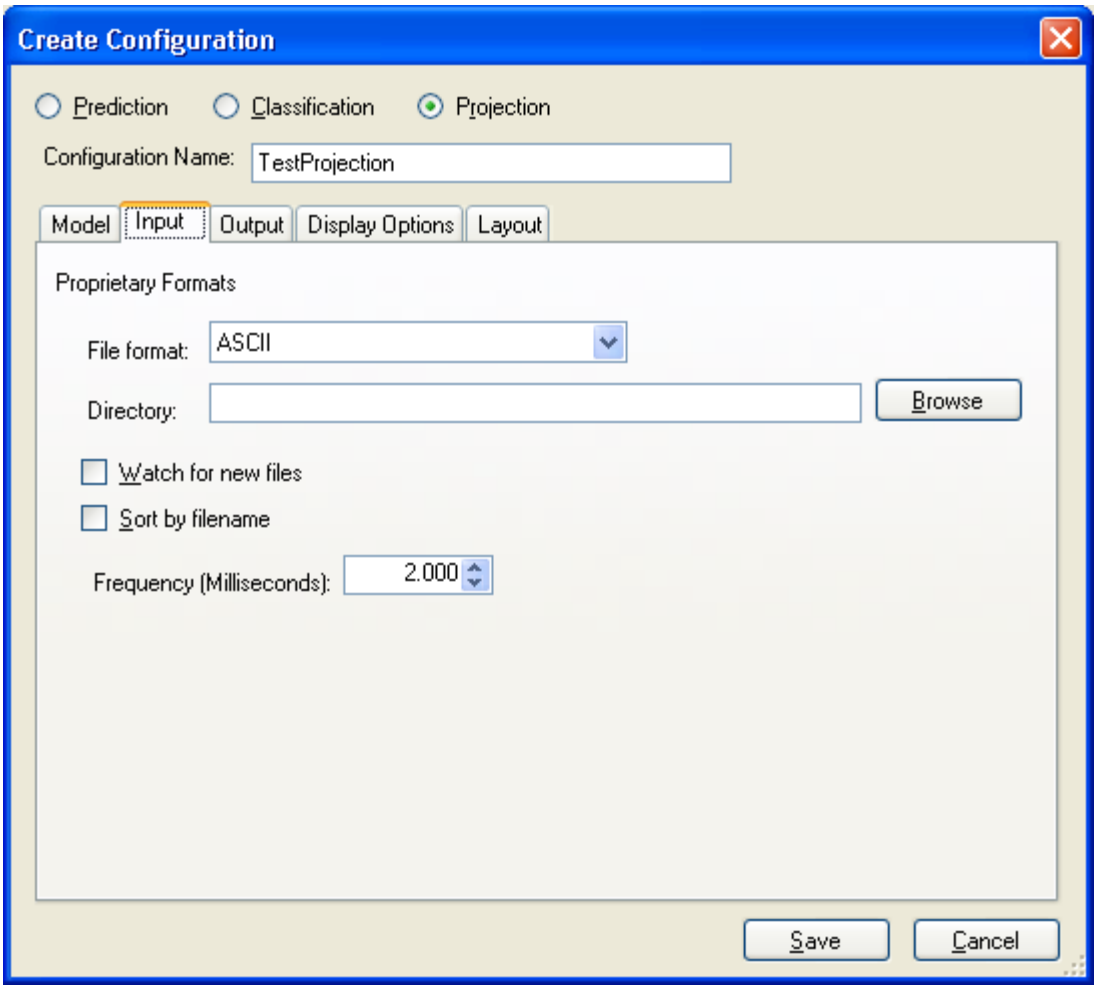

Figure 28 - Input tab for Projection

Watch for New Files

If this option is selected, the projection process is notified whenever a new file is added to the *Input* directory. The new file is loaded and processed once any previous projections have been completed.

This option is for what is known as *asynchronous* mode of operation. When this mode is set the other two options, *Sort by file name* and *Frequency* cannot be set.

Sort by File Name

If this option is selected, all existing files in the *Input* directory are sorted and loaded sequentially in alphabetical order. Projection is performed on the samples in their sorted order.

Frequency

The numeric *Frequency* box can be used to provide the frequency (in milliseconds) at which the application should poll the *Input* directory for new data.

The Output tab

The information required for performing projection and storing the results are defined in the *Output* tab, (see Figure 29Figure 22 for an example for a projection configuration method)

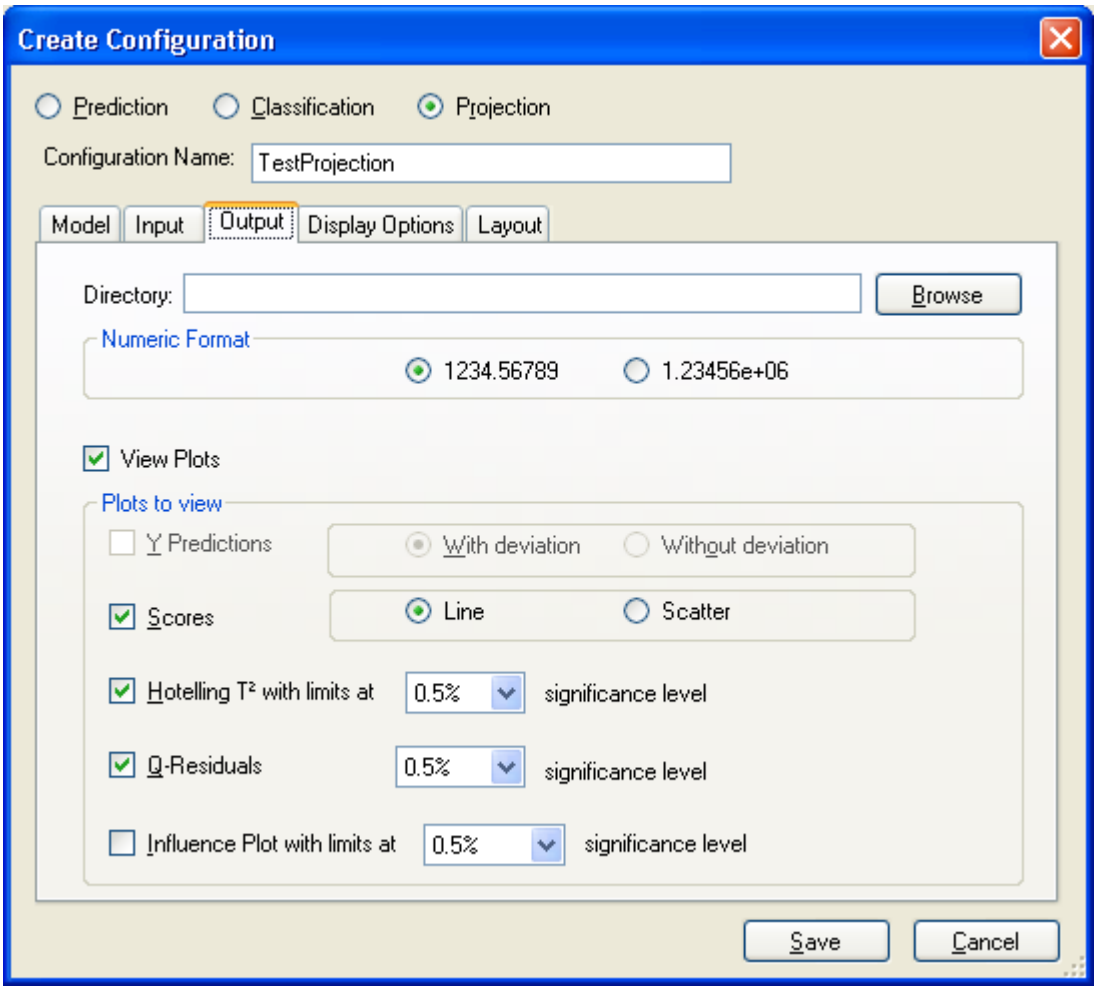

Figure 29 - Output Tab for Projection

Output directory

The *Output* directory defines the path for the output files which include the results file.

Numeric Format

The *Numeric Format* box provides the option to print the numeric results in floating point format (12345.6789111) or exponential format (1.234568e+06). Depending on the selection, the results are stored in floating point or scientific notation.

Plots to view (Projection Configuration Methods Only)

A user can select which diagnostic plot(s) to display during process monitoring. One or more of the following plots may be displayed

- Scores (line or 2D-scatter plot)
- Hotelling's T^2-statistics with limits at a specified significance level
- Q-Residuals at a specified significance level
- Influence Plot with limits at a specified significance level

Note: If the view plots option is selected, the plots are displayed during process monitoring, the outputs of projections are written directly in the output directory.

The Display Options tab

This tab is available for prediction configuration methods only. An example is provided in Figure 30.

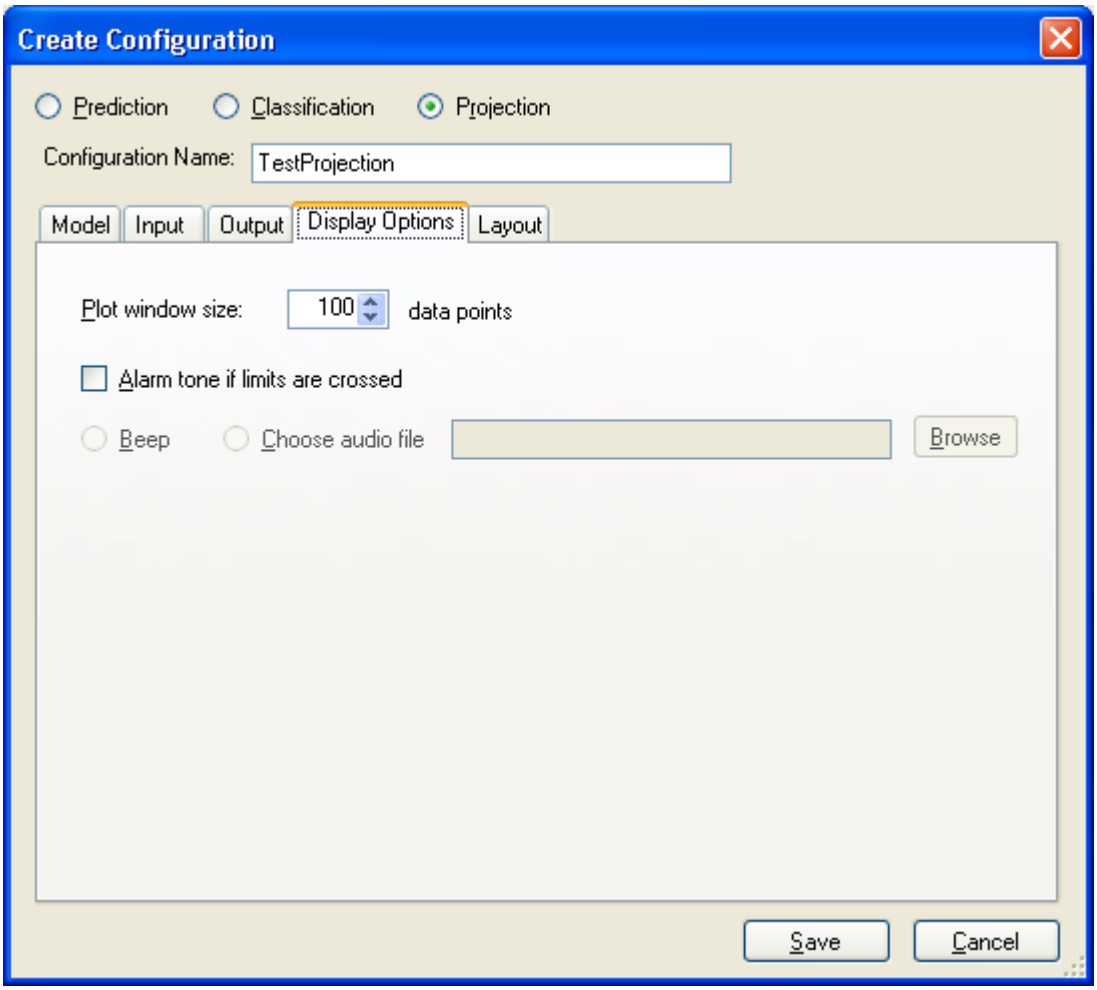

Figure 30 - Display options tab

Plot Window Size

The maximum number of data points to be displayed in the plots is defined here.

Alarm tone if Limits Are Crossed

An audible alarm is sounded whenever the process deviates from target conditions if this option is selected. The alarm can be used from the Operating System beep sound or an audio file can be specified for alarm.

The Layout tab

For configuration methods using projection models, a user can select any layout from the list of nine shown in Figure 33. The layout should have the same number of panes as there are plots selected in the *Output* tab.

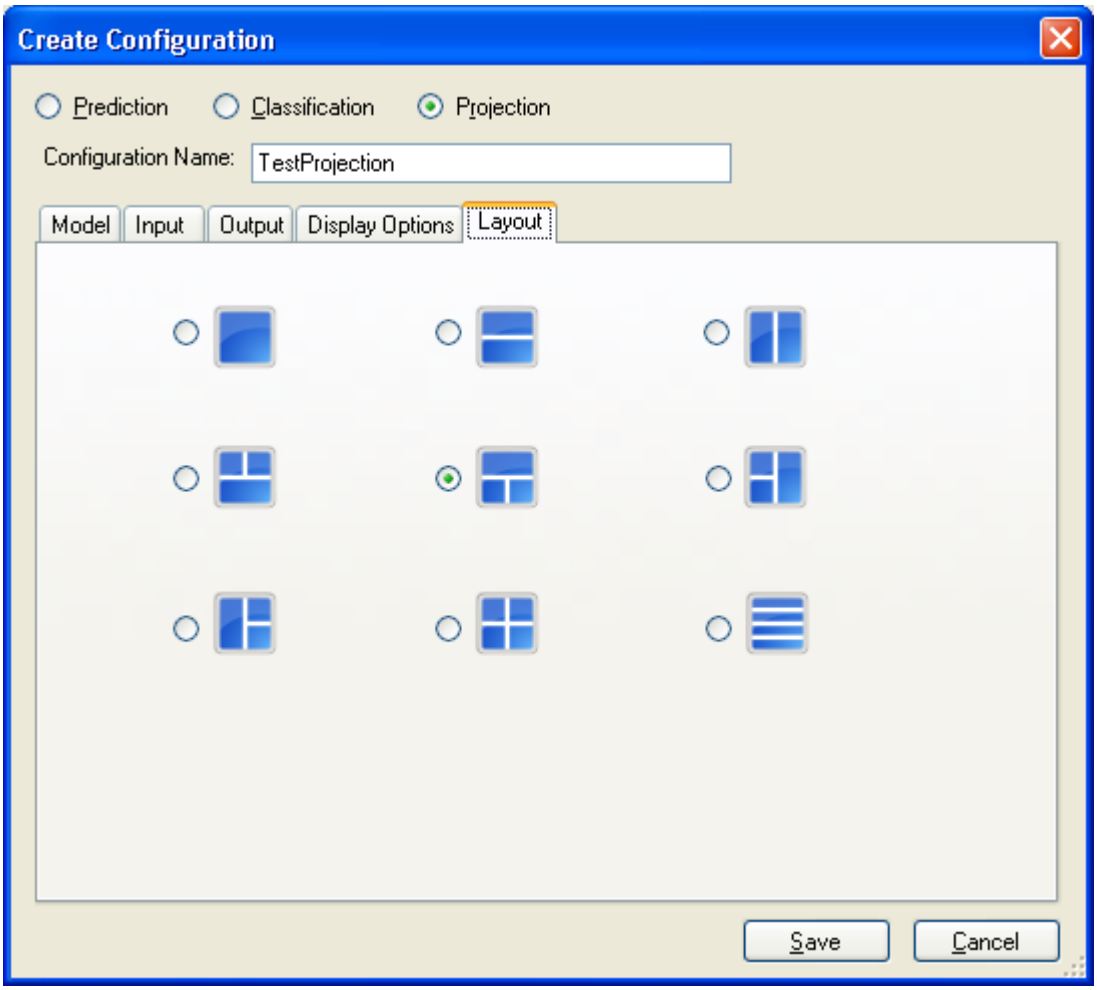

Figure 31 - Layout tab

Save Configuration Method

All of the settings (options) chosen by the user are saved as a *Configuration method*.

Configuration method names can be any alphanumeric text (including some special characters like underscore '_', hyphen '-'and opening and closing brackets '('and ')') but not a space character.

Click the **Save** button to save the configuration method into the *Configuration Navigator*. The configuration method appears in the configuration navigator with the name it was saved as.

3.5 Configuration Method Modifications

In general, sections 3.5.1 through 3.5.3 can be performed on any configuration method available from the configuration navigator. Setting of passwords for protecting methods is discussed in section 3.5.4. If a configuration method is password protected, the functions described in sections 3.5.1 through 3.5.3 cannot be performed unless the password is known to the user.

3.5.1 Duplicate a configuration method

Existing configuration methods can be duplicated in order to make small changes without deleting previous settings. Access this option through **File –> Configuration –> Duplicate** or use the designated toolbar button ( ). See Figure 32.

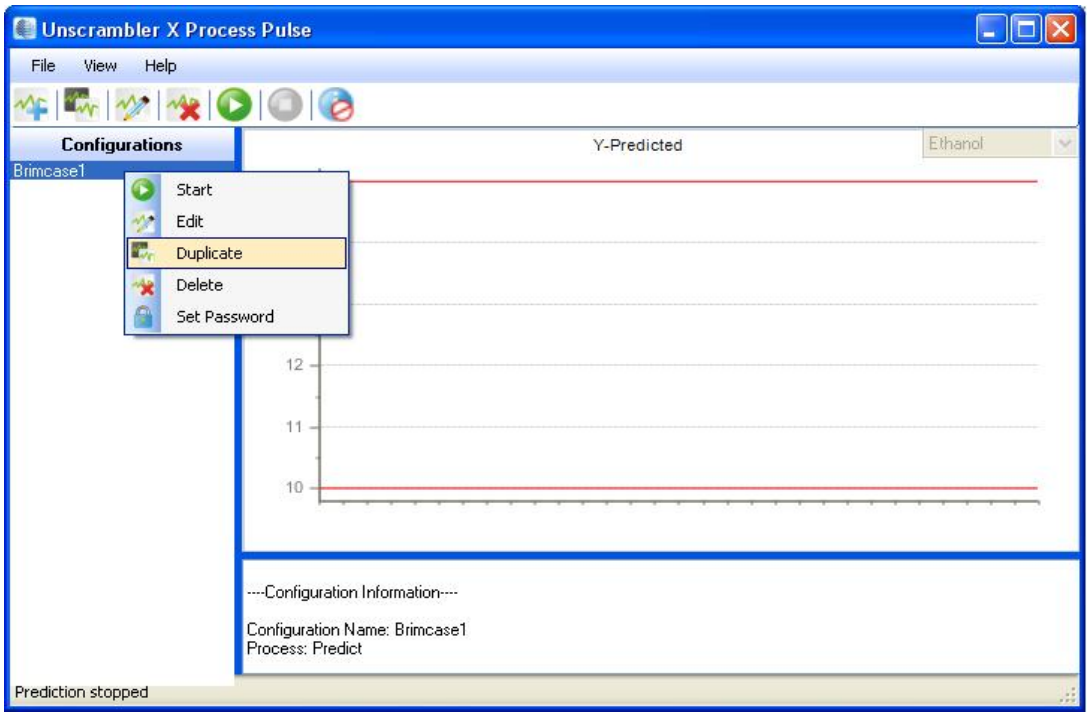

Figure 32 - Duplicate Configuration Option

A unique name must be provided to the duplicated method in order to save it to the configuration navigator. If no new name is provided, the existing method name is indexed based on the number of duplications. See Figure 33 for an example.

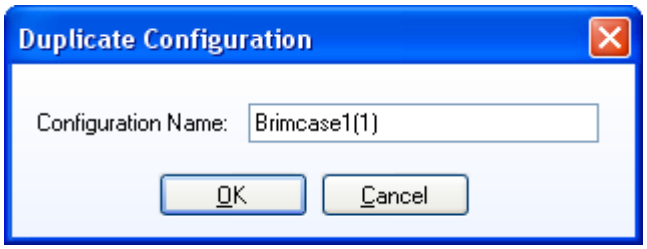

Figure 33 - Duplicate Configuration Name

3.5.2 Editing a configuration

Existing configuration methods can be modified by highlighting a specific method from the configuration navigator list and choosing **File –> Configuration –> Edit** or using the designated toolbar button ( ). See Figure 34.

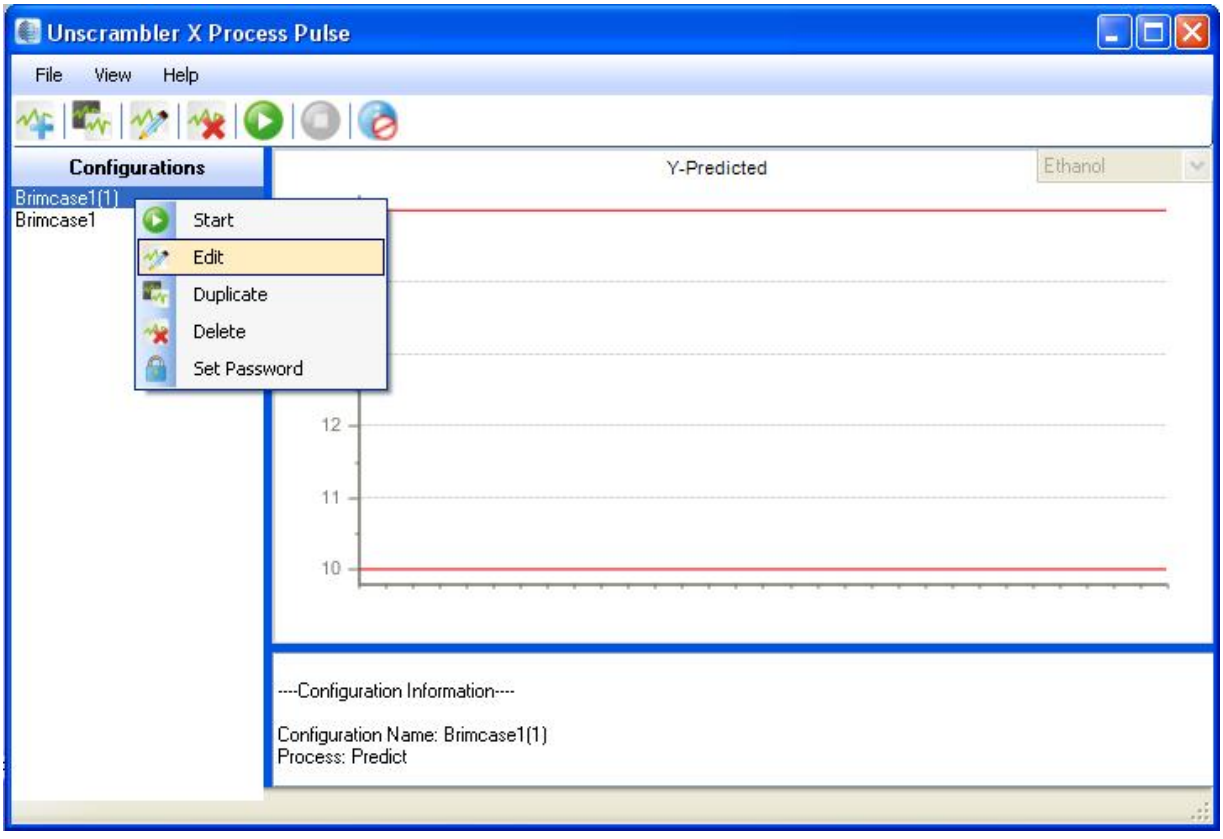

Figure 34 - Edit Configuration Option

3.5.3 *Delete a configuration*

Any configuration that is no longer required can be removed by highlighting the method in the configuration navigator and choosing **File –> Configuration –> Delete** or by clicking the **Delete** button ( ). See Figure 35.

Caution: The configuration method will be removed from the Configuration navigator as well as from the disk. A warning similar to that shown in Figure 36 will be provided before a configuration method can be deleted.

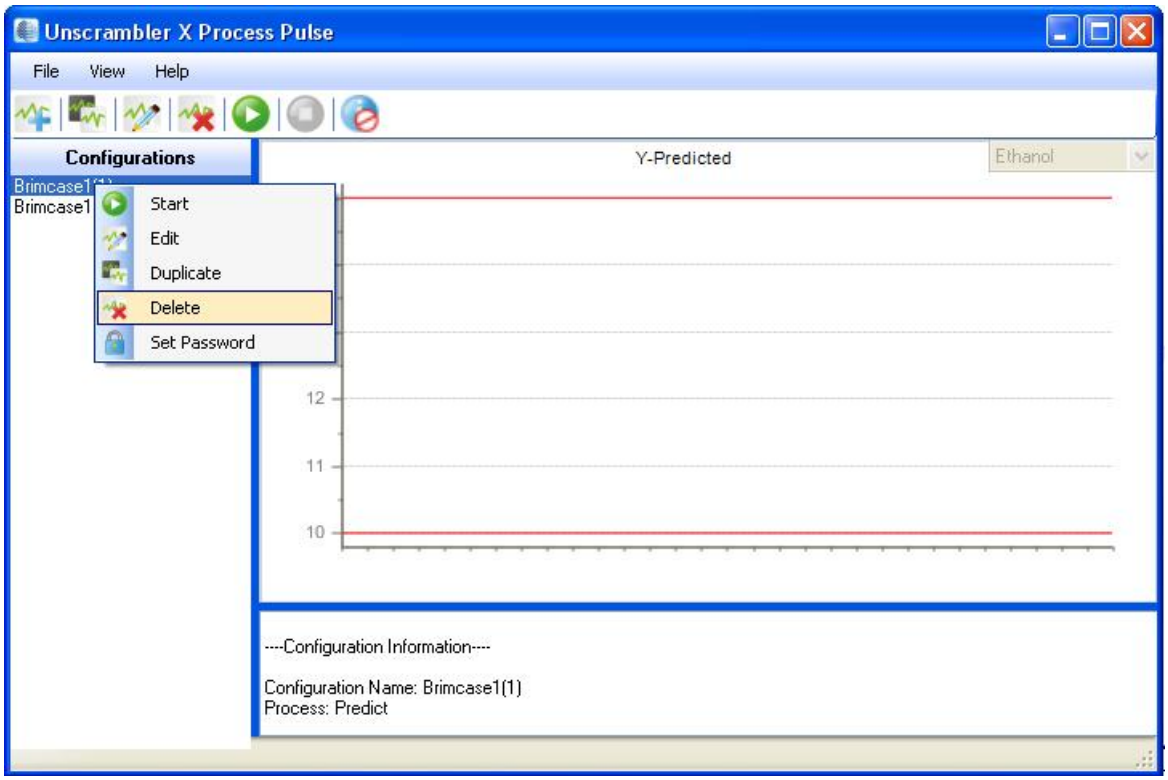

Figure 35 - Delete Configuration option in Menu

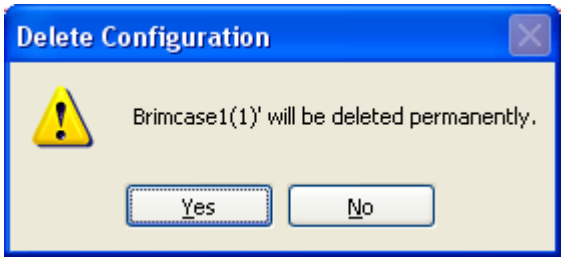

Figure 36 - Confirmation message for deletion

3.5.4 *Setting Passwords for Configuration Methods*

A configuration method can be password protected in Unscrambler X Process Pulse for the prevention of any tampering. This is optional and was implemented to meet the basic compliance requirements of some organizations. The user should re-enter the password for confirmation.

Caution: It is a user's responsibility to record a password in a secure location in the event of forgetting it. Unscrambler X Process Pulse has no password recovery mechanism implemented. If such a requirement is necessary, contact your local CAMO Software office for more details.

The configuration methods, protected by password, cannot be edited, deleted or duplicated without providing the correct password. See Figure 37, Figure 38 and Figure 39.

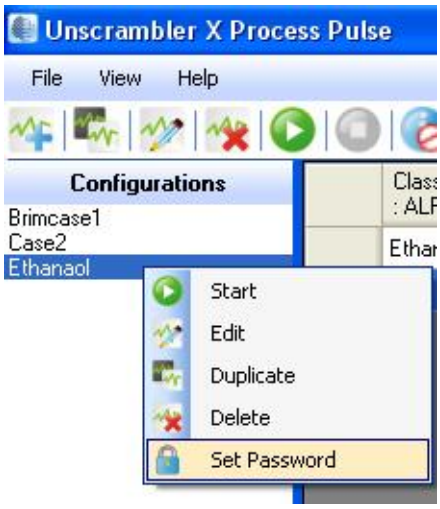

Figure 37 - Set Password for Configuration

Figure 38 - Password Dialog

Figure 39 - Confirmation of Password

3.6 *Run Prediction / Classification/ Projection Configuration Methods*

To use a configuration method for real time analysis, select the configuration method from the configuration navigator and click on the **Start** button in the toolbar ( ) (Figure 40) or from the menu **File-> Start** (Figure 41).

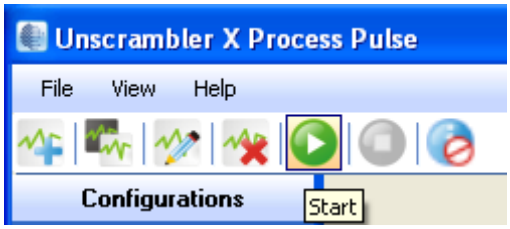

Figure 40 - Option for starting a Configuration Method

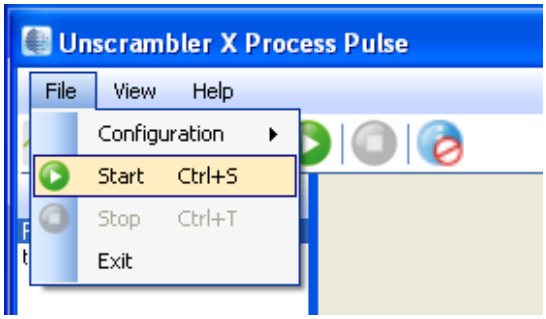

Figure 41 - Option for starting Configuration

If the configuration is running with ASCII data as the input file format, a window requesting the number of row headers in the data will appear. Enter the values for the number of row headers in the file, and the number of rows to be skipped (see Figure 42)

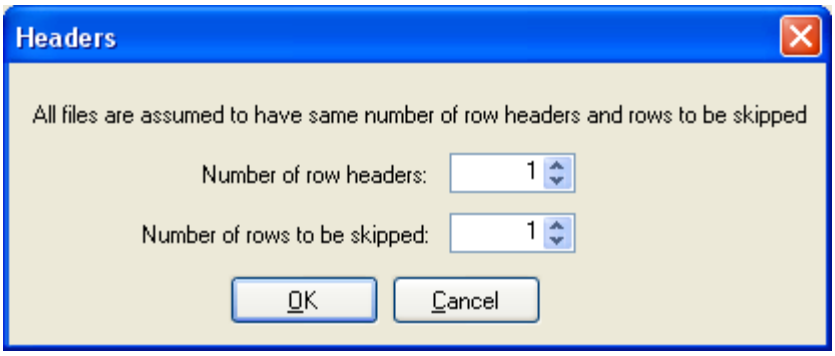

Figure 42 - Headers for ASCII Files

When the **Start** button is clicked, the user should enter the details of the batch/operation in the *Annotation* dialog as shown in Figure 43. Comments are added to the final results folder and the Batch ID entered can be searched for using the *Data History* option described in section 3.10.

Figure 43 - Annotation Dialog

When the process monitoring starts the status of the prediction or classification or projection progress is displayed in the bottom left corner of the main window (following normal windows software conventions).

3.7 Running a Classification

The output view for a classification is the *Membership table*, which has a column for each class model, and a row for each new sample being classified. The sample class is given by a one (1) in the column that corresponds to the sample's class membership, with zeros (0) in the other columns (See Figure 44).

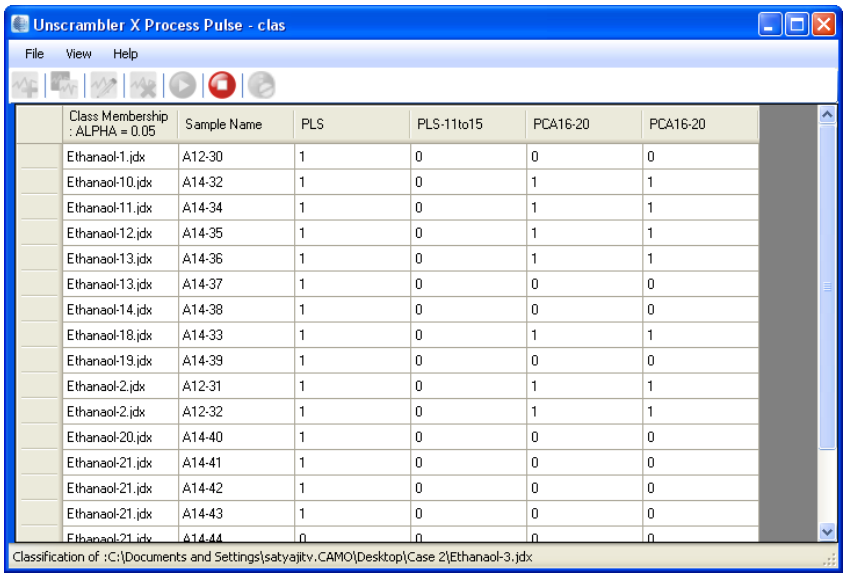

Figure 35 - Example of a Class Membership Table

3.8 Stop prediction/classification/projection configuration method

To stop a prediction or classification or projection configuration method, press the **Stop** button ( ) in the toolbar, or from **File -> Stop**. Once this is performed, the results are saved to the *Output* files. Numerical results can be viewed by selecting **View -> Data History** (more details on Data History are provided in section 3.10)

3.9 Plot View

The pre-configured plots, setup in the configuration method, are the default outputs for prediction or projection methods. When a configuration method is started a plot window appears, see Figure 44 A maximum of four plots can be displayed at one time. The upper and lower limit for the Y-Predicted values, set in the *Output* tab, will be displayed. The Y-Predicted values which cross these limits are highlighted in red in the plot. As a new sample is read in, the corresponding Y-Predicted value is plotted in real-time. By default a scrolling graph is displayed with points disappearing beyond the Y-axis as set in the configuration method.

A user can right click on any of the plots during the prediction/classification/projection procedure and select the **Save Plot** option to save it in any of the .EMF, .BMP, .GIF, .TIFF, .JPEG, or .PNG formats. Alternatively, the **Save All Plots** option can be selected to save all the plots as a single image file in formats described above.

A user can copy any of the plots to the clipboard for use in third party applications such as Microsoft Word.

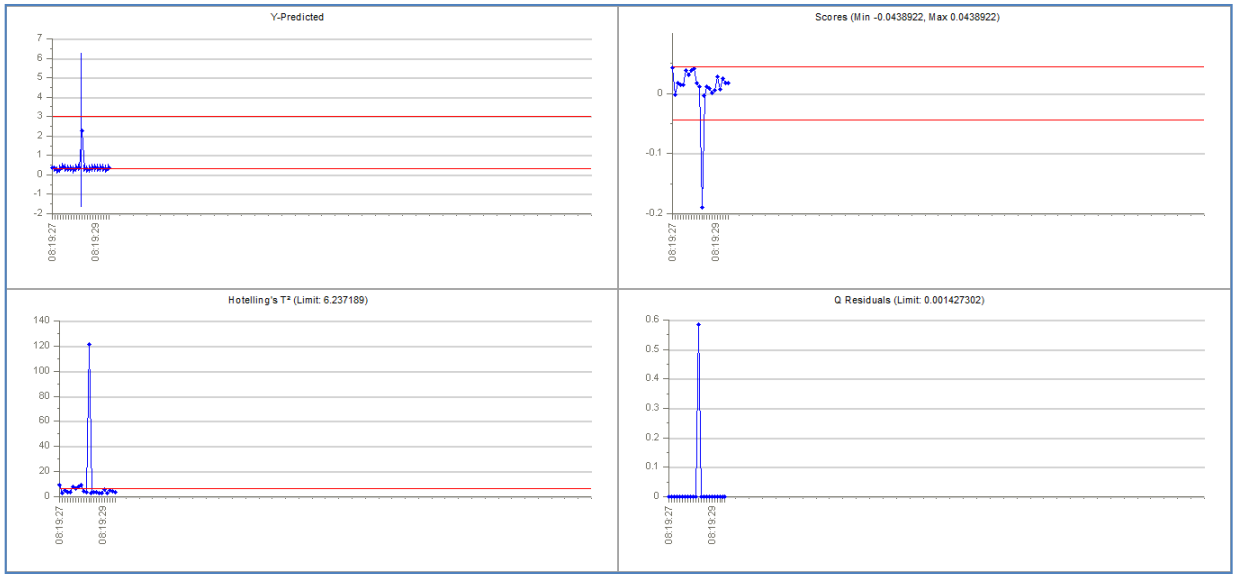

Figure 44 - Plot View as defined in the Configuration Method

3.10 View Data History

All output data, irrespective of prediction / classification/ projection, are stored and displayed in the *Data History* form. Results data are displayed based on the selected configuration. The *Data History* form has 3 sections (see Figure 45).

1. **Search** – select any configuration method available from the drop down box to view the result set. Also available are search by date/time which will help in retrieving results between time frames.
2. **Result Set** – based on the search mode, the result set generated for the configuration method will be displayed, ordered by time & date. A configuration method may have more than one result associated with it since, every time it is started, a new result set is created and relevant data are stored in it.
3. **Display** – click on any item in the result set and the data available in the result set will be displayed. This display is read only and can be used to view the output of a configuration at an instance of time. The contents can be copied and pasted from the display. Values can also be sorted by double-clicking on the column to sort on.

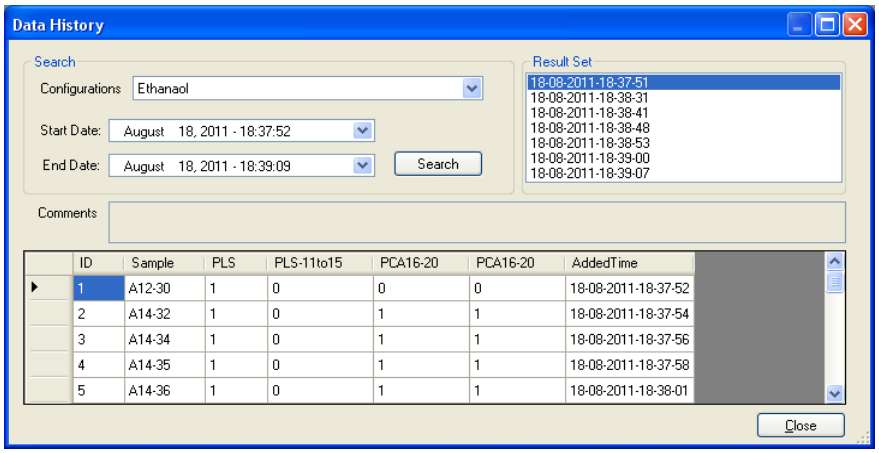

Figure 45 - Data History

3.11 *Options Dialog*

Individual Plot Settings

Settings for individual plots can be customized from the *Options* dialog (Figure 46 - Options Dialog). These options can be customized only when a *Theme* is not selected. Plots can be formatted for the following options:

1. Show/Hide Y axis Gridlines
2. Show/Hide Plot header
3. Configure the color of lines
4. Configure the thickness of lines
5. Configure the color of limit lines
6. Configure the size of points to be displayed. If the size is set to zero, the points on the line are not shown
7. Configure axis labels to show either *Names* or *Numbers*

If a *Theme* is selected, the following options can be configured:

1. Show/Hide Y-axis gridlines
2. Show/Hide Plot header
3. Configure axis labels to show either *Names* or *Numbers*

General Options

Number of points in scores plot

Set the number points to be shown in a *Scores Scatter* plot. The default number of points shown is 250.

Size of output file

This option allows a user to set limitations on the size of the *Output* file. By default 20 MB is the set size. A user can change this option as desired. If the size of the output file exceeds this limit, a new file is created in the *Output* directory

Antialiasing

Enables smoother graphics, which present better on computer displays, but may look blurry in print format.

Connection lines in scores

Enables connected lines for points in scores scatter plots.

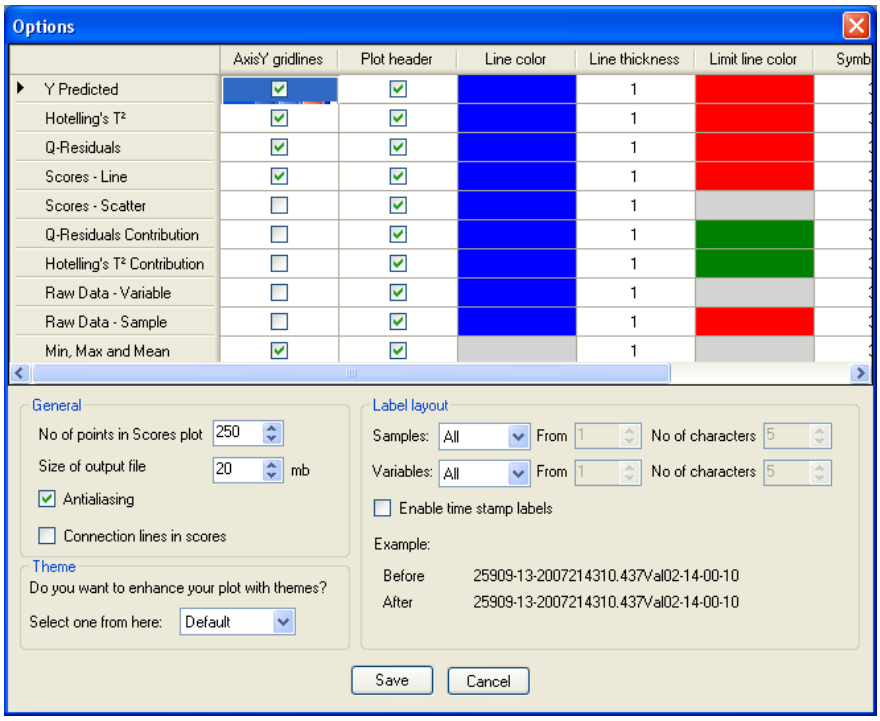

Figure 46 - Options Dialog

Label Layout

For the *Axis Label* of samples and variables the text can be edited for instance by customizing the name, such as only having part of the name displayed. For this option use the drop-down list in *Label layout for Samples and Variables*. By default the first 10 characters of sample and variable names are shown in a plot.

Enable time stamp labels

This option can be used to show the time stamp for samples. This time stamp indicates the time when the sample was read from the specified folder and is the time set on the specific computer running Unscrambler X Process Pulse

Selecting a Theme

Plots can be customized based on user preference by selecting various predefined themes. A user can choose from four themes available.

3.12 *Audit Trail*

The entire audit trail of Unscrambler X Process Pulse can be found from **View -> Audit Trail** (See Figure 47).

Figure 47 - Audit Trail Option

The *Audit trail* list provides information for all the actions performed in Unscrambler X Process Pulse (see Figure 48)

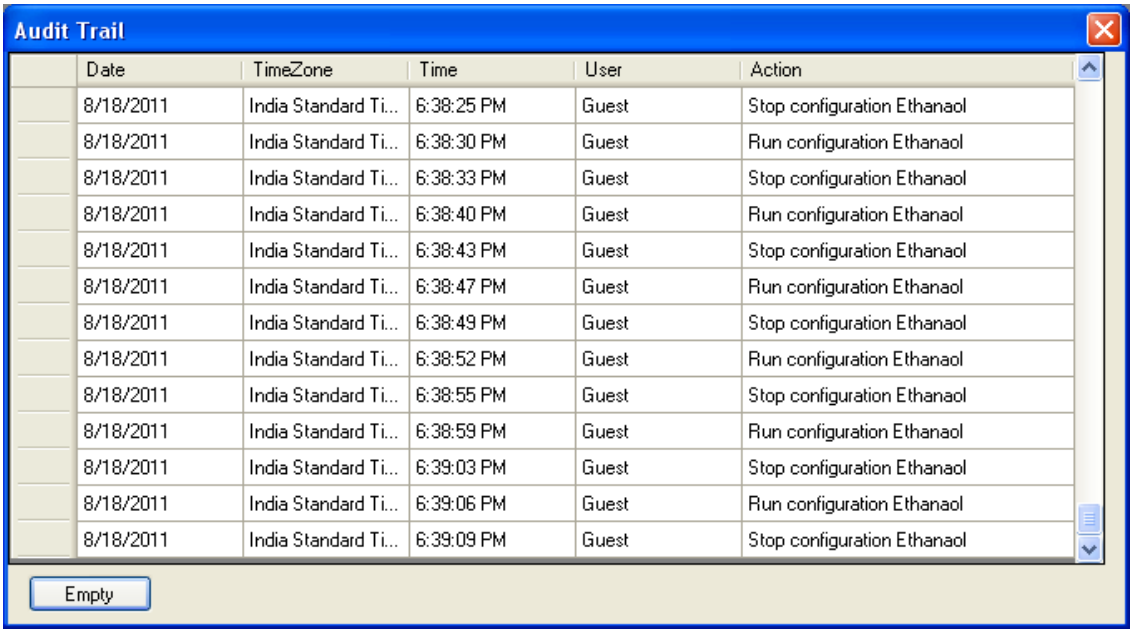

Figure 48 - Audit Trail Dialog

3.13 *Modify License*

The license of Unscrambler X Process Pulse can be upgraded using the option **Help -> Modify License**, (see Figure 49)

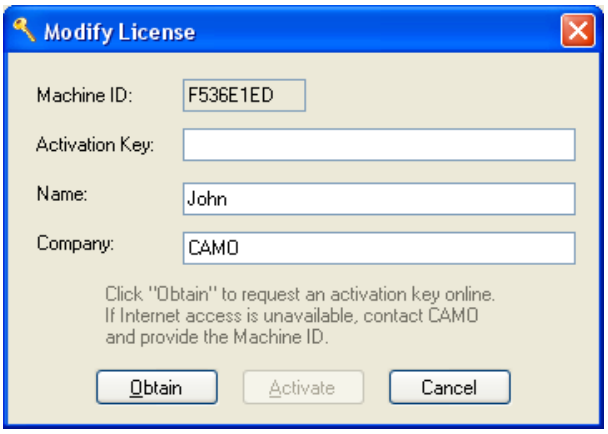

Figure 49 - Modify license dialog

4 Plots for Prediction and Projection

Note: All plots can be zoomed into using the scroll button on a mouse.

4.1 Y-Predicted Plot

This plot is applicable only for prediction configurations. This plot is disabled for projection configurations

The Y-predicted plot is a simple univariate run chart of the response (Y) being predicted from the multivariate model assigned to the configuration method. This provides real-time values for measurements plotted as a function of sample (time). This plot can be displayed with limits (if they are set in the *Display Options*, see section 3.11.2). The name of the response plotted is shown in the upper right corner. If a model can predict more than one response, values for others can be displayed by selecting them from the drop-down list at the top of the plot. The Y- predicted plot can be displayed in a number of variants, as designated in the configuration *Output*. Additional information about the raw data for a given sample and for variables can be accessed by double clicking on the Y-predicted plot to access drill-down plots (see section 4.1.5).

The following options are available for Y-predicted plots

1. *Y-Predicted plot without deviation*: This is a plot of the predicted Y values vs. sample identification (time) and is autoscaled for the Y-values. This plot shows the number of points set in the *Options* menu. Once this number of points has been exceeded, the plot scrolls by replacing the first result with the last one. See Figure 50 for an example of this plot.

2. *Y-Predicted plot with deviation:* Y-values with deviation are plotted if designated in the *Output* tab. The deviation is an indicator of whether the predicted results are reliable, as it is a measure of the samples' residual and leverage relative to the calibration data. The deviation is computed from the following expression

$$yDeviation = \sqrt{ResYValVar\left(\frac{ResXValSamp_{pred}}{ResXValTot} + Hi + \frac{1}{I_{cal}}\right)\left(1 - \frac{a+1}{I_{cal}}\right)}$$

Where

ResYValVar is the residual Y-variance from the validated residual.

ResXValSamp – is the residual X-validation variance that comes from the prediction of the new sample

ResXValTot – is the average residual X-validation in the model.

H_i is leverage of the new sample predicted relative to the calibration set

I_{Cal} is number of calibration samples

a is the number of factors/components in the calibration model

See Figure 51 for an example of this plot type.

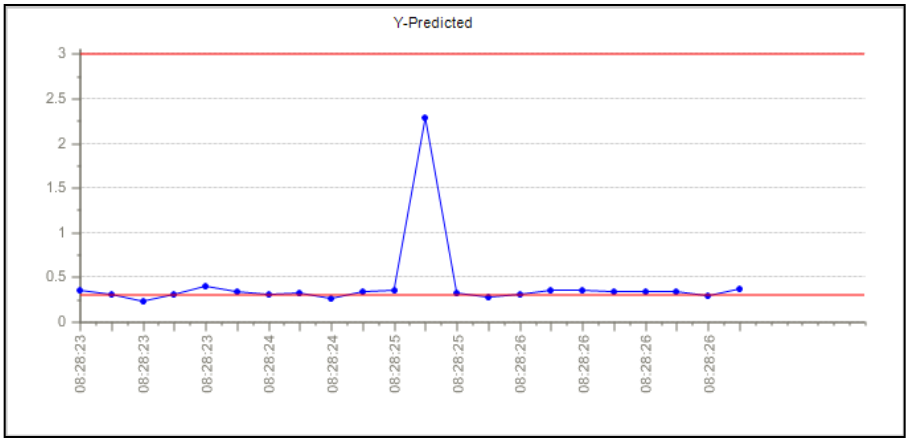

Figure 50 - Y-Predicted plot with upper and lower limits without deviations

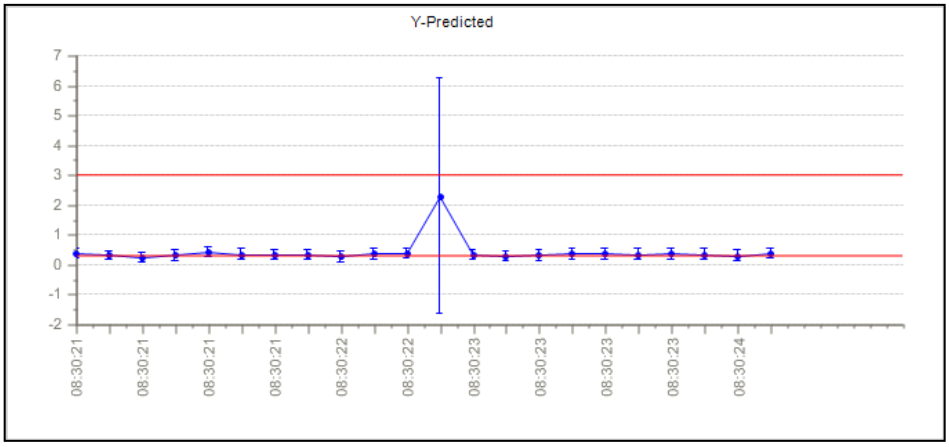

Figure 51 - Y-Predicted plot with upper and lower limits with deviations

4.2 Scores Plot

The scores space from a multivariate prediction model is a measure of the total variance in the data with respect to a calibration set. A plot of the scores, though not quantitative, provides a means to trend the variance in sample data. It can also serve as a visualization of the similarity of samples with respect to each other, when viewed either as a line or a 2D scatter plot.

The following options are available for scores plots

1. *Scores Line plot:* The scores line plot is displayed for the highest number of PCs in a model for each new sample predicted, and is shown with the Hotelling T^2 limit lines at that number of PCs in the model. The upper and lower limits for the Hoteling T^2 lines are based on the points where the overall confidence ellipse would cross the PC axes, if the scores were plotted as a 2D graph. To change the view to another PC, select the desired PC from the drop-down list in the upper right hand corner. See Figure 52 for an example line scores plot.

2. *Scores Scatter plot (with Hotelling's T^2 ellipse):* When the scores are plotted as a scatter plot, the default plot is of PC1 vs. PC2. Other 2-D scatter plot combinations can be chosen from the drop-down menu. In this view (with the *Default* theme) the last point predicted is shown as a larger green dot. Samples outside the limits are displayed as red dots. The last 10 points are shown in blue, and older points are shown in grey for the default settings of the plot. The points color scheme is changed based on the *Theme* selected. See Figure 53 for an example of a 2-D scatter scores plot.

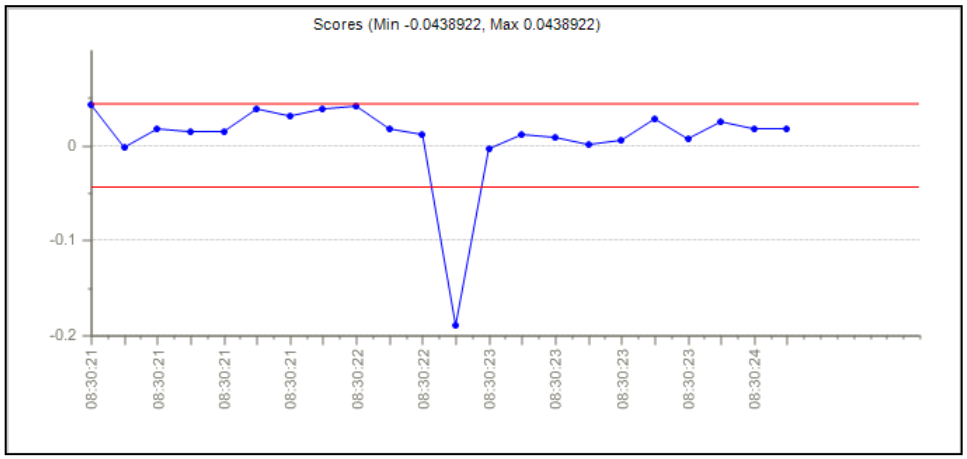

Figure 52 - Scores Line plot with limits

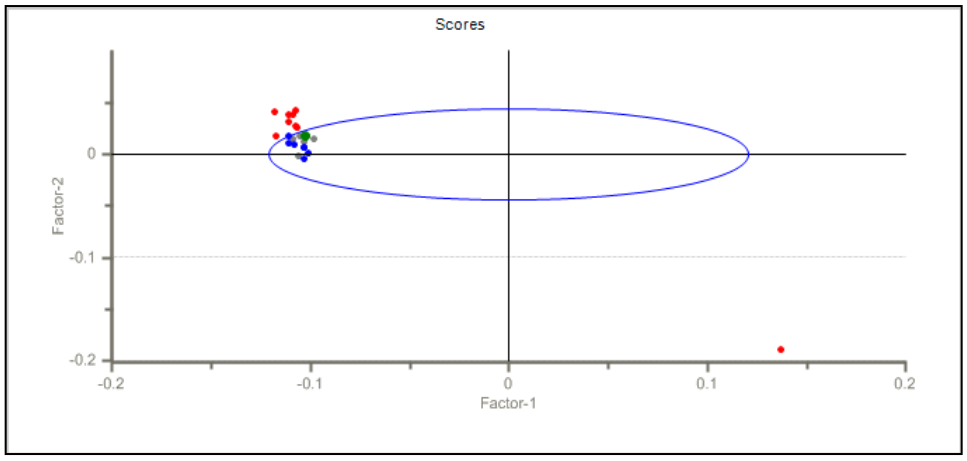

Figure 53 - Scores Scatter plot with Hotelling's T2 Ellipse

4.3 Hotelling's T^2–statistics with limits

During process monitoring outlier statistics are powerful tools for identifying if samples are different to those used in the calibration set. Such outlier statistics are used for detecting process deviations, potential process upsets or measurement issues. The Hotelling's T^2 limit is calculated based on the calibration samples, and based on a user-specified significance level (0.1, 0.5, 1.0, 5.0, 10.0, and 25.0%). The limit

serves as outlier detection for newly measured samples and those exceeding the limits are deemed outliers. Such samples are well explained by the model but represent extreme variation and should be further investigated. Contribution plots for the Hotelling's T^2 plot can aid in finding the root cause of an outlying sample. See Figure 54 for an example of the Hotelling's T^2 statistics plot with limits.

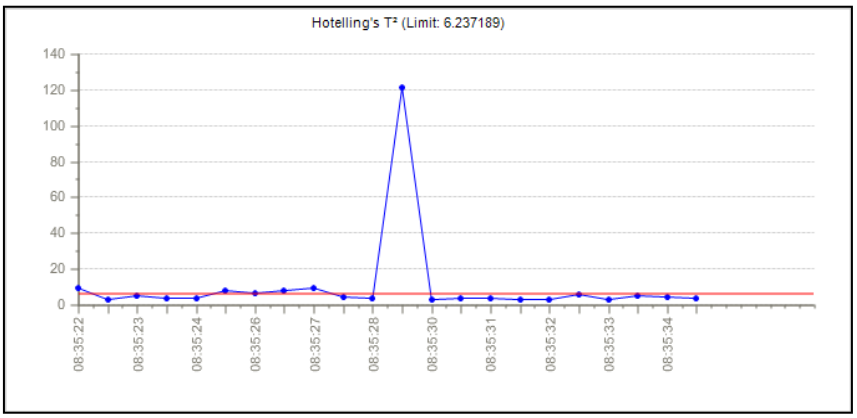

Figure 54 - Hotelling T2 Plot with limits

4.4 Q-Residuals Plot

Another valuable outlier detection statistic in process monitoring is the Q residuals, which are related to the variance in the variables (e.g. a sample spectrum) that is not explained by the model being used. Samples whose Q-residual values exceed the limit line might be considered as outliers and should be further investigated to identify the root cause of the difference. Figure 55 provides an example of a Q-Residuals plot.

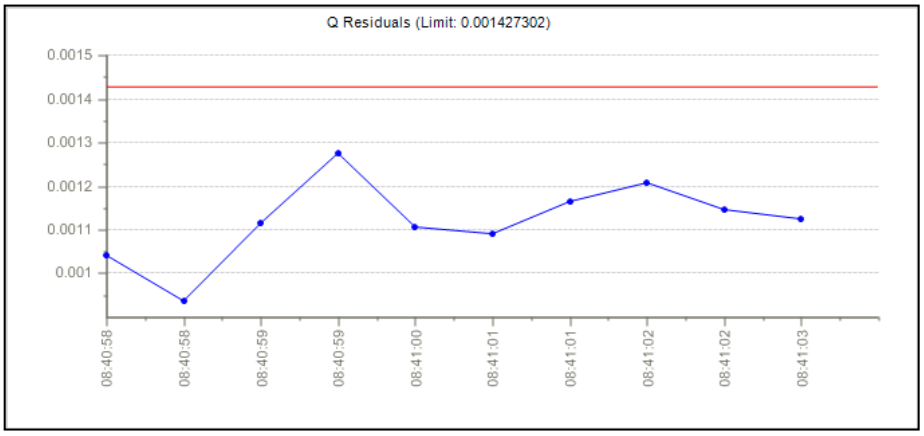

Figure 55 - Q-Residuals Plot with limits

4.5 Raw Data Drill-down Plot

In the situation where more information is required about a predicted sample, this can be obtained by double-clicking on a sample point in the *Y-predicted* or *Scores* plot. This will open a two-plot view consisting of the *Raw Data*, and the *Min/Max/Mean* plot for the selected point.

The *Raw Data* plot can be shows for Raw data and processed data using the icon *"Pre-processed data"* in upper right corner(

). This is useful to see the data in raw and pre-processed format. For large spectra the points can be either shown or hidden using the *"Hide points"* icon (). The plots can be changed to bar plot using "*Change plot type to Bar*" icon ().

The *Min/Max/Mean* plot (which is a variation on a box and whisker plot) is used to isolate any variable(s) that are different with respect to those of the calibration set. This plot can be shown with data centered and scaled by clicking the icon in the upper right corner (

), which is particularly useful if the variables are of different units and scales .See Figure 56 for an example of this plot.

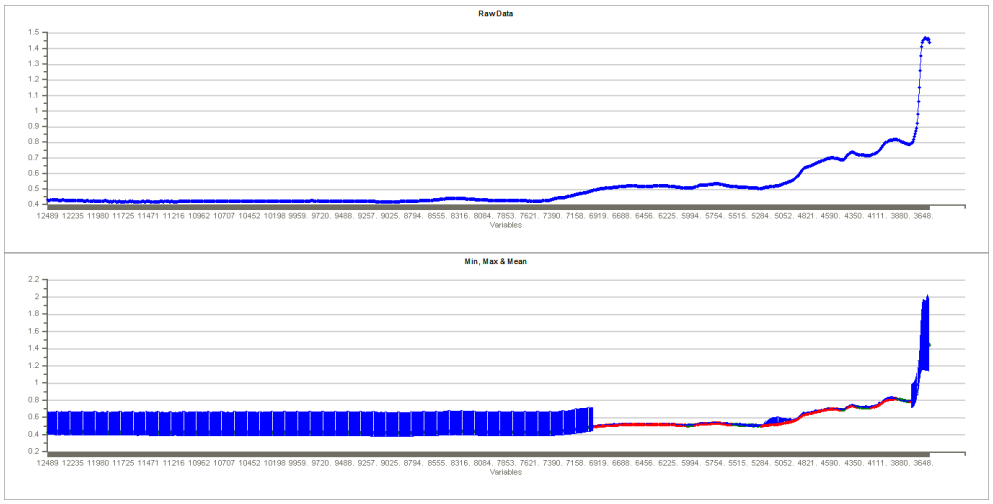

Figure 56 -Raw Data plot compared to Calibration data

4.6 Raw Data Double Drill-down Plot

A further drill-down plot of the values for a selected variable and the 10 samples around can be displayed by double-clicking on a variable in the raw data plot. The name of the variable being displayed is shown in the window header. The value for the selected sample is shown as a hashed bar (in bar plot view), with the other samples shown as filled bars. Lines for the minimum and maximum values of the variable in the calibration set area also on the plot, and the values in the plot title. The plot may also be displayed as a line plot, and the selected sample point will be displayed larger than the other points in the plot (see Figure 57)

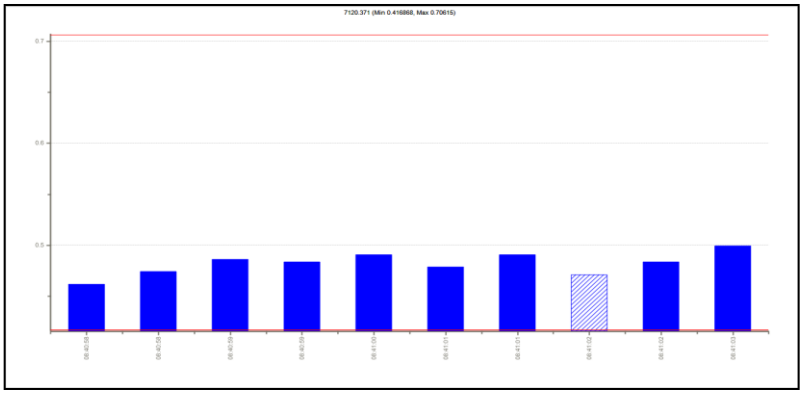

Figure 57 - Double drill-down for raw data plot

4.7 *Contribution Plot for Hotelling's T^2-Plot*

Contribution plots are used in process monitoring to indicate the contribution of each variable to a measured statistic such as the Hotelling's T^2 or Q residuals. They aid in determining which variable(s) contribute to a sample being outside the limits for the statistic. High contribution values may be indicative of a problem with that variable, and are therefore useful in fault detection.

The contribution plot is opened by double clicking on a sample point in the Hotelling's T^2 or Q Residuals plot which opens two contribution plots in a new window. The upper plot shows the contribution of each variable to the Hotelling's T^2 (as a bar) in the order of the variables. A line on the plot shows the model's average for the Hotelling's T^2 values. This shows how much each variable for the selected sample differs from the model's average values – a good means of identifying what may be plausible variables related to faults. If both the Hotelling's T^2 and Q-Residuals are chosen in the output display, contribution plots for both will open.

The contributions of each variable for a selected sample are shown, and can be sorted in ascending/descending order. The bar plot can be changed to a line plot by toggling the icon in the upper right corner ( ) (Figure 58)

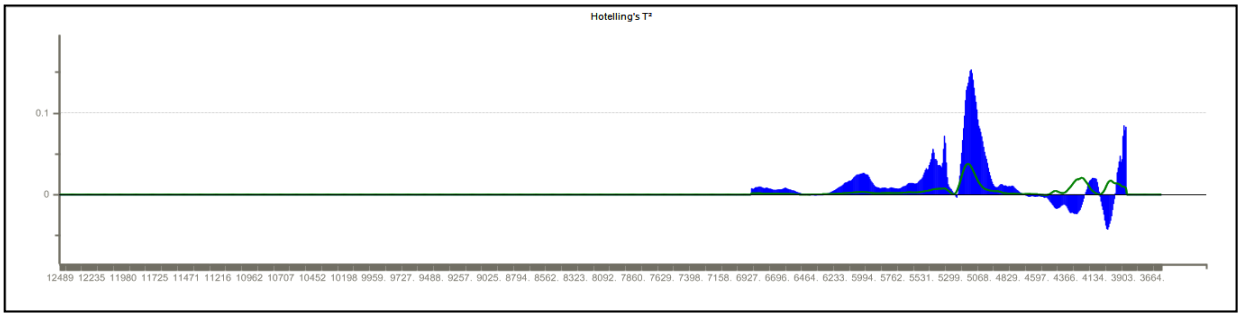

Figure 58 - Contribution plot for Hotelling's T2-statistics

4.8 Contribution Plot for Q-Residual Plot

The contribution plot for the Q residuals is opened by double clicking on a sample point in the Q Residuals or Hotelling's T^2 plot. The lower of the two contribution plots show the contribution of each variable to the Q residuals (as a bar) in the order of the variables. A line on the plot shows the model's average for the Q residual values. This shows how much each variable for the selected sample differs from the model's average values – a good means of identifying what may be plausible variables related to faults.

The contributions for each variable for the selected sample are shown, and can be sorted in ascending/descending order. The bar plot can be changed to a line plot by toggling the icon in the upper right corner ( ) (See Figure 59).

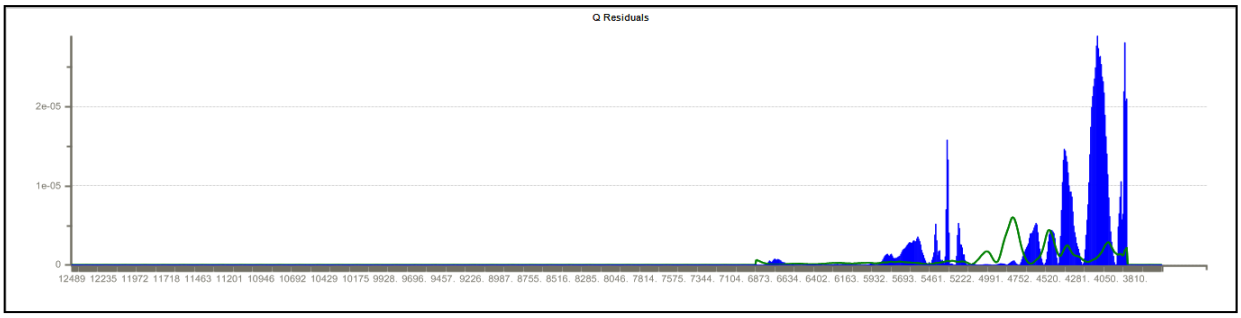

Figure 59 - Contribution plot for Q-Residuals

4.9 Influence Q-Residual Plot

Another valuable outlier detection statistic in process monitoring is the Influence Q-Residual Plot. This plot shows the Q-residual X-variance vs. Hotelling T^2. The Q-residual is the sum of squares of the residuals over the variables for each object.

This test serves the purpose of finding outliers in terms of the distance to the model space, i.e. residual distance. Given the model $X = TP' + E$, then the Q-residuals for the objects in X are computed from the diagonal of EE'.

A critical value of the Q-residual can be estimated from the eigenvalues of E, which can be approximated to a normal distribution Jackson and Mudholkar, 1979. This is the horizontal red line.

The Hotelling T^2 statistic describes the distance to the model center as spanned by the principal components.

A plot of the Q-residual distance vs. Hotelling T^2 is referred to as the Influence Q-residual plot and is suited to spot samples which may be regarded as outliers as being too extreme in the model sense or being "something else". See Figure 60.

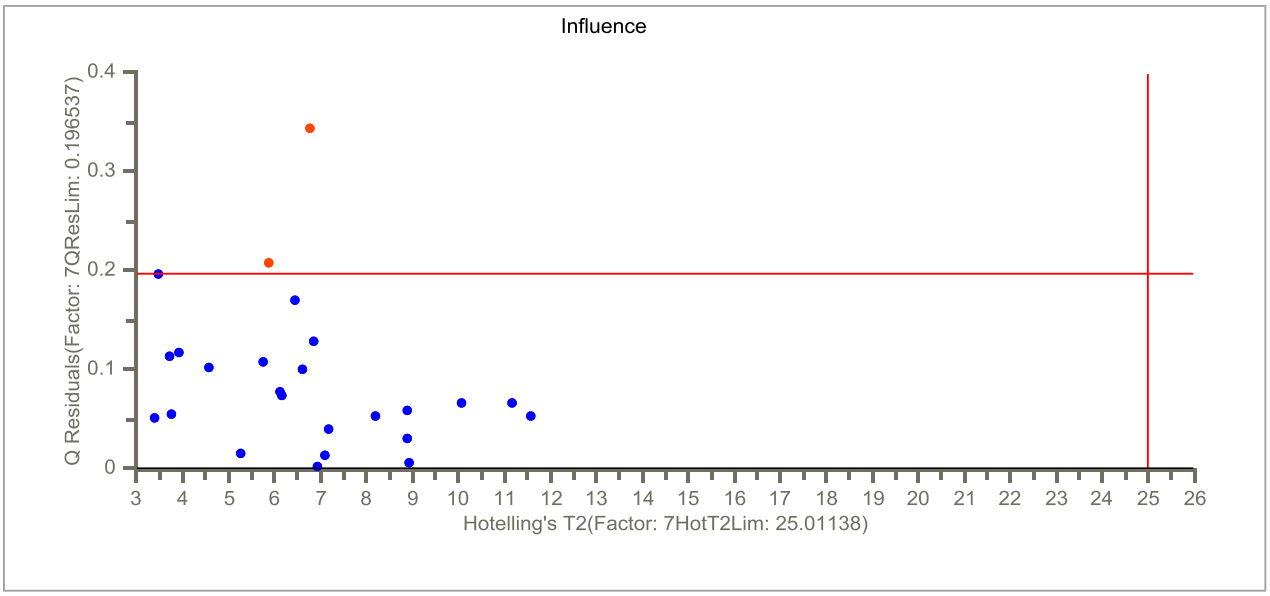

Figure 60 - Influence Plot

5 Output files

Up to five files are generated when a configuration method is run, and are found in the *Output* folder. The *Analysis Result* file in Unscrambler X Process Pulse format is in the output folder, while the other files are in a subfolder with the name of the configuration method.

1. Unscrambler X Process Pulse results (Configuration name dd-mm-yyyy-hh-mm-ss.upp)
2. The configuration summary file (ConfigSummary_dd-mm-yyyy-hh-mm-ss.csv)
3. The results file (configuration name-dd-mm-yyyy-hh-mm-ss.csv)
4. An error log (configuration name_ErrorLog_dd-mm-yyyy-hh-mm-ss.txt)
5. An alarms file (Alarms_configuration name_dd-mm-yyyy-hh-mm-ss.csv

For Classification only two output files are created: the *.upp and the results file in the folder with the configuration method name.

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